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THE MAGNETIC ROTATION SPECTRUM OF SULFUR DIOXIDE IN THE 3000Å REGION

A THESIS

Presented to

The Faculty of the Graduate Division

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John Lafayette Hardwick

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THE MAGNETIC ROTATION SPECTRUM OF

SULFUR DIOXIDE IN THE 3000Å REGION

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SUMMARY

This work was directed toward an analysis of the rotational fine structure of the magnetic rotation spectrum of sulfur dioxide in the region near 3000Å. This system has long defied analysis by conventional techniques of absorption spectroscopy, and the clarity of the coarse band structure of the magnetic rotation spectrum provided promise of our understanding the excited electronic state in some detail.

Measurements of the magnetic rotation spectra of SO_2^{16} and SO_2^{18} were made photographically at high resolution, transcribed onto magnetic tape as digitized data, and displayed graphically using a Univac 1108 computer equipped with a Calcomp plotter. The transition frequencies were then assigned, and the excited state term values were fitted to a symmetric rotor energy formula.

The results of the analysis strongly indicate that the excited electronic state is a linear or nearly linear $^1B_1$ component of a Renner-split $^1\Delta_g$ state, the other component of which is the ground electronic state. Coupling of the $^1B_1$ electronic state to high-energy vibronic levels of the ground electronic state gives rise to a nonvanishing expectation value for the electronic orbital angular momentum.

Five bands of each isotopic species have been analyzed, and between 40 and 100 lines of the ^pP and ^rR branches have been fitted to within 0.1-0.2 cm^{-1} rms deviation. The rotational constants and band origins are presented, and some conclusions are drawn regarding the structure and vibrational assignment of the excited state.

CHAPTER I

INTRODUCTION AND BACKGROUND

The near ultraviolet spectrum of sulfur dioxide was first studied by Henri (1), and later by Watson and Parker (2) and Clements (3). Their qualitative results were that there were three main regions of absorption: a strong absorption system beginning at about 2300Å, a moderately strong system centered around 3000Å, and a very weak feature at 3800Å.

Clements resolved the vibrational structure of the 3000Å system and denoted the strong features beginning about 3130Å by the letters A, B, C, ..., attributing these features to a single progression in the excited state bending mode, ν_2'. He assigned the weak features at 3800Å as "hot" bands of the 3000Å system.

Metropolis and Beutler (4) showed, through a temperature-dependent study of the spectrum, that the 3800Å bands constitute a separate system. Merer (5) has performed partial rotational and vibrational analyses of low-lying bands of this system, and Brand, Jones, and diLauro (6) have completed detailed rotational analyses proving that the system arises from a transition from the ground state to a $^3B_1$ excited state.[1] This system also exhibits a magnetic rotation spectrum which was discovered

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1. In accordance with (7), z is assigned as the C_{2v} axis, x perpendicular to the plane of the molecule, and y parallel to the figure axis of the (prolate) almost-symmetric top. Thus, B_1 transforms as a rotation about the figure axis and as a translation perpendicular to this axis.

and studied by Dr. B. S. Snowden at Georgia Tech in 1964.

Metropolis (8) attempted a vibrational analysis of the 3000Å system, in which he attributed the strong A, B, C ... features to transitions to accidentally degenerate vibronic states. Furthermore, on the basis of a simple valence force field model for the excited state, as well as the red-degraded K-structure, Metropolis assigned the excited state a bond angle of about 100°. On this basis, as well as on the basis of a comment by Merer (5) that the bands of this system are of parallel type, the excited state has been assumed by many authors to have $^1B_2$ symmetry.

The predictions of molecular orbital theory are, however, quite different from the conclusions reached by Metropolis. The simple arguments of Walsh (9) and of Mulliken (10) predict that the lowest-lying excited singlet electronic state will have B_1 symmetry, and that it will have a bond angle larger than that of the ground state. Since these theories have proven to be of quite general usefulness in describing the low-lying excited electronic states of triatomic molecules, most recent authors (11) have chosen to refer to the excited state as $^1B_1$, even though the complexity of the rotational structure has heretofore precluded an analysis to confirm or refute this assignment.

The MO predictions may be thought of in terms of a Walsh diagram (Figure 1) for a molecule with 18 valence electrons. The <u>linear</u> molecule will have a ...$(\pi_u^*)^2$ ground electron configuration, leading to states of $^3\Sigma_g^-$, $^1\Delta_g$, and $^1\Sigma_g^+$ symmetry. As the molecule bends, the π_u^* orbitals are split into orbitals of a_1 and b_1 symmetry, giving rise to the states ... $(a_1)^2\ ^1A_1$, ... $(a_1)(b_1)\ ^1B_1$, ... $(a_1)(b_1)\ ^3B_1$,

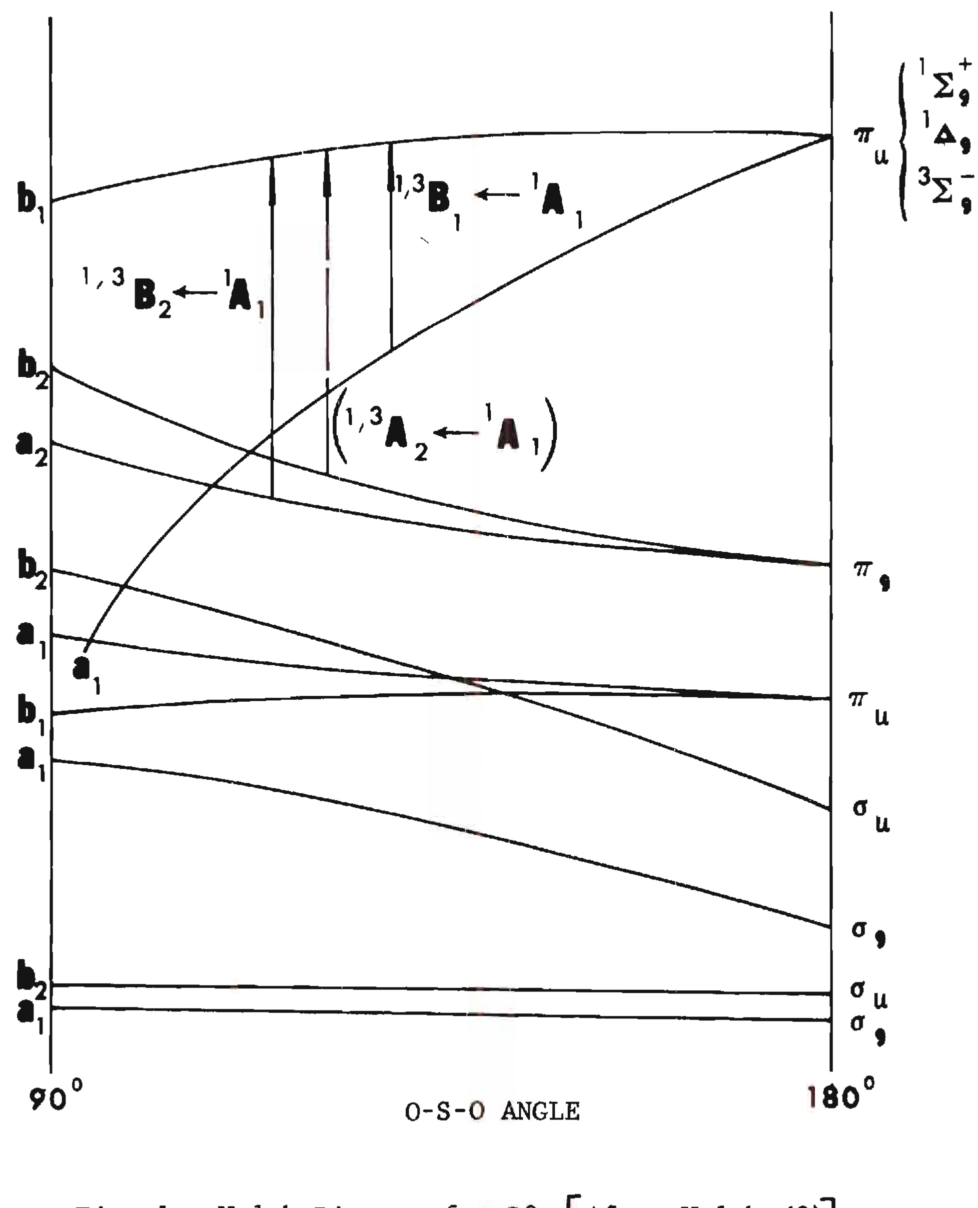


Fig. 1. Walsh Diagram for SO_2 [After Walsh (9)].

and ... $(b_1)^2\ {}^1A_1$. The first two states correlate with the ${}^1\Delta_g$ state of the linear conformation; the third correlates with the ${}^3\Sigma_g^-$ state; and the last state correlates with the ${}^1\Sigma_g^+$ state (see Figure 1). Transitions to the ${}^1A_1$ (${}^1\Sigma_g^+$) state have not been observed; this state represents a two-electron promotion from the (bent) ground state.

The strong absorption system at 2300Å has been shown by Srikameswaran and Brand (12) to arise from a ${}^1B_2 \leftarrow {}^1A_1$ transition, corresponding to a promotion of an electron from an a_2 to a b_1 orbital. The corresponding triplet system has not been observed, nor has the (forbidden) promotion of an electron from the higher b_2 to the lowest b_1 orbital.

The 3400-2600Å system, in addition to having a complex rotational structure, exhibits other anomalous behavior indicative of mixing with another electronic state.

Kusch and Loomis (13) observed a strong magnetic rotation spectrum for this system, contrary to expectations for a singlet-singlet transition of a nonlinear triatomic molecule. Since the intensity of the system (roughly 3 orders of magnitude more intense than the ${}^3B_1$ system) seems to preclude a spin-forbidden transition, the system must acquire its ability to interact with the magnetic field through mixing with some other state.

Fluorescence experiments have, on the whole, yielded results even more complex than absorption and magnetic rotation experiments. Greenough and Duncan (14) and Douglas (15) found the lifetime of the singlet emission to be approximately 42 μsec at zero pressure, a value almost two orders of magnitude greater than that calculated from the integrated absorption coefficient.

Furthermore, the rate of collisional deactivation of the singlet excited state is nearly equal to the collision frequency (16), a fact consistent with the argument that there is an unusually efficient mechanism for mixing the excited electronic state with the ground state.

Douglas interpreted the increase in lifetime as evidence of mixing with another electronic state. Strickler and Howell (16) have shown that the only state with a high enough density of vibrational levels to cause an effect of the observed magnitude is the ground state.

Thus it appears clear that the fluorescence data alone imply a strong mixing with the ground state. This result is rather surprising, since vibronic mixing of $^1B_1$ and $^1A_1$ states is not allowed for bent triatomic molecules; mixing is possible only through a Hamiltonian involving the total rovibronic symmetry of the two states.

More recently, Sidebotton et al. (17) have observed that both the zero-pressure lifetime and the quenching coefficient appear to be a function of vibrational excitation of the excited singlet state. These authors report a lifetime of 36 ± 4 μsec for the molecule "prepared" by excitation at 2662Å and a lifetime of 18 ± 6 μsec for a singlet molecule at vibrational equilibrium. The basis of their conclusions is their observation of a non-exponential decay of the singlet system.

Gardner (18) has suggested that the fluorescence results may be accounted for by Renner-Teller coupling of the rovibronic levels of the ground and excited electronic states. This coupling would also account for the magnetic rotation spectrum exhibited by this system, as well as the recent observation by Brand and co-workers (19) of a strong Zeeman effect in many lines of the system.

CHAPTER II

EXPERIMENTAL

Spectra were observed using a modified Jarrell-Ash 3.4 meter Ebert-mount spectrograph. Low resolution spectra were recorded using a 30,000 line per inch grating blazed at 13^{o} in the first order. Dispersion for this grating was approximately 1.2Å/mm. High resolution spectra were recorded using a 7,500 line per inch grating blazed at 59^{o} in the 18th-21st orders. This experimental apparatus has been described in detail elsewhere (20).

Orders were sorted using an order-sorter designed in this laboratory by S. W. Twiggs and constructed by the author. The order-sorter consisted of two plane mirrors and a concave grating, all kinematically mounted (see Figure 2). The first mirror in the optical path was mounted on a movable arm whose position could be set using a micrometer to vary the angle of incidence of light on the grating. Collimated light was reflected from the movable mirror to the grating; the dispersed light was then reflected by the second mirror and focused on the spectrograph slit. The dispersion of the order-sorter was parallel to the spectrograph slit and, hence, perpendicular to the dispersion of the spectrograph grating.

All spectra were recorded photographically using Kodak 103-aO photographic plates. The light source was a high pressure mercury arc.

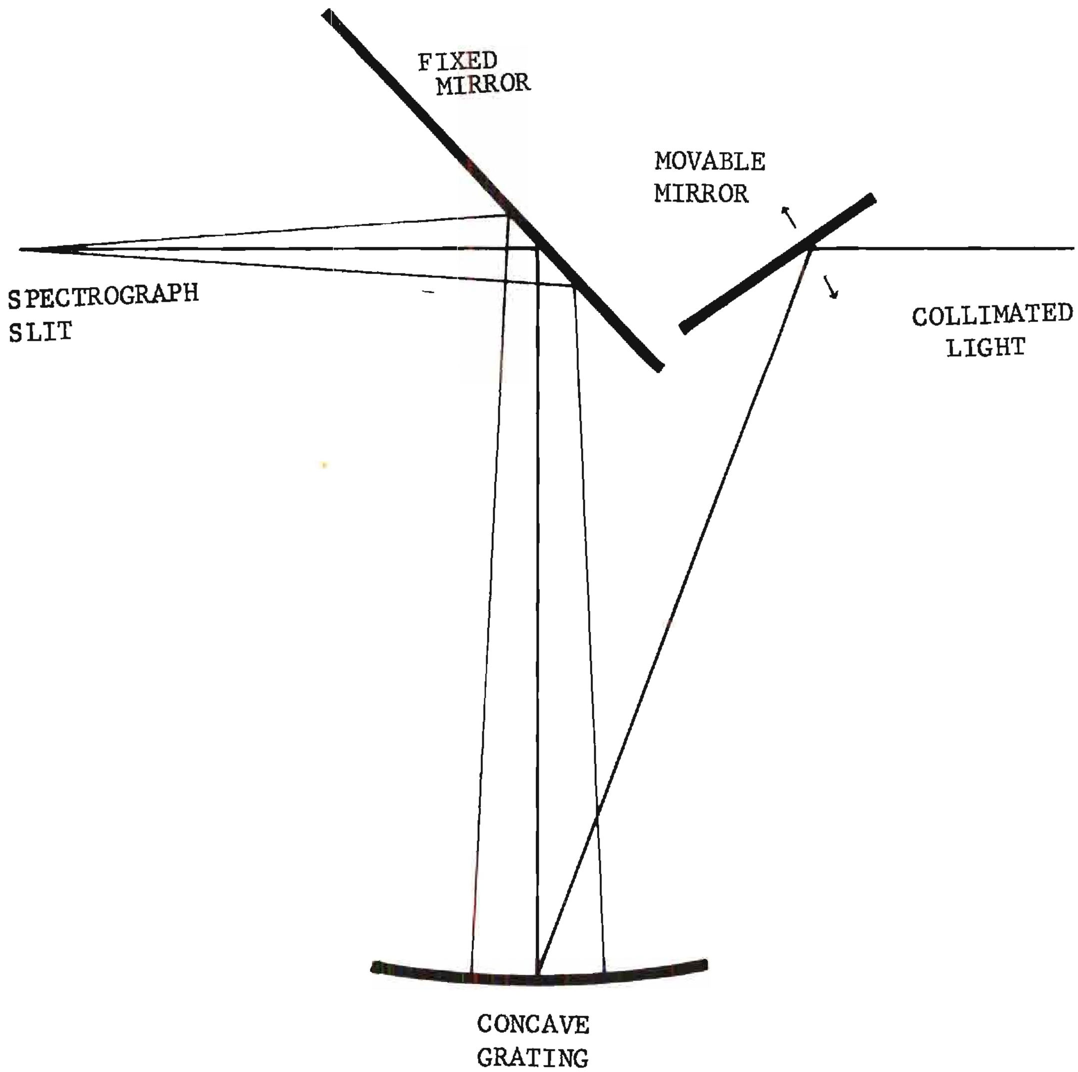


Fig. 2. Optical Diagram for the Order Sorter.

Magnetic rotation was observed using a longitudinal field of approximately 2.5 kG. Cells 65 cm long and 2.5 cm in diameter fitted with strain-free quartz windows were used to contain the sample.

Iron calibration lines were produced by means of a microwave discharge in FeI_3 (21). Vacuum wavelengths for many iron lines have been given to eight significant figures by Stanley and Meggers (21). Air wavelengths for many additional lines have been tabulated to seven or eight significant figures by Striganov and Sventitskii (22). The former reference was used as a primary standard, and air wavelengths of the same lines tabulated in the latter reference were used to construct an effective refractive index curve for air as a function of wavelength. This curve was used to calculate consistent vacuum wavelengths from the latter reference.

Spectra were transcribed from photographic plates using a Leeds & Northrup model 6700-A2 scanning densitometer. This instrument focuses the image of a straight-filament lamp onto the photographic emulsion; an image of the emulsion is then focused on a slit and projected onto a pair of photoresistors.

A 45 volt DC potential from a dry cell battery was applied to the photoresistors, and the current flowing through the circuit (on the order of 10^{-7} amperes) was monitored and amplified using a Keithley 610B electrometer (see Figure 3).

The electrometer signal was converted into a frequency modulated signal using a Hewlett-Packard model 2212A voltage-to-frequency converter. The range of frequencies was adjusted by adjusting the gain of the electrometer and by applying a variable resistance across the input to the voltage-to-frequency converter.

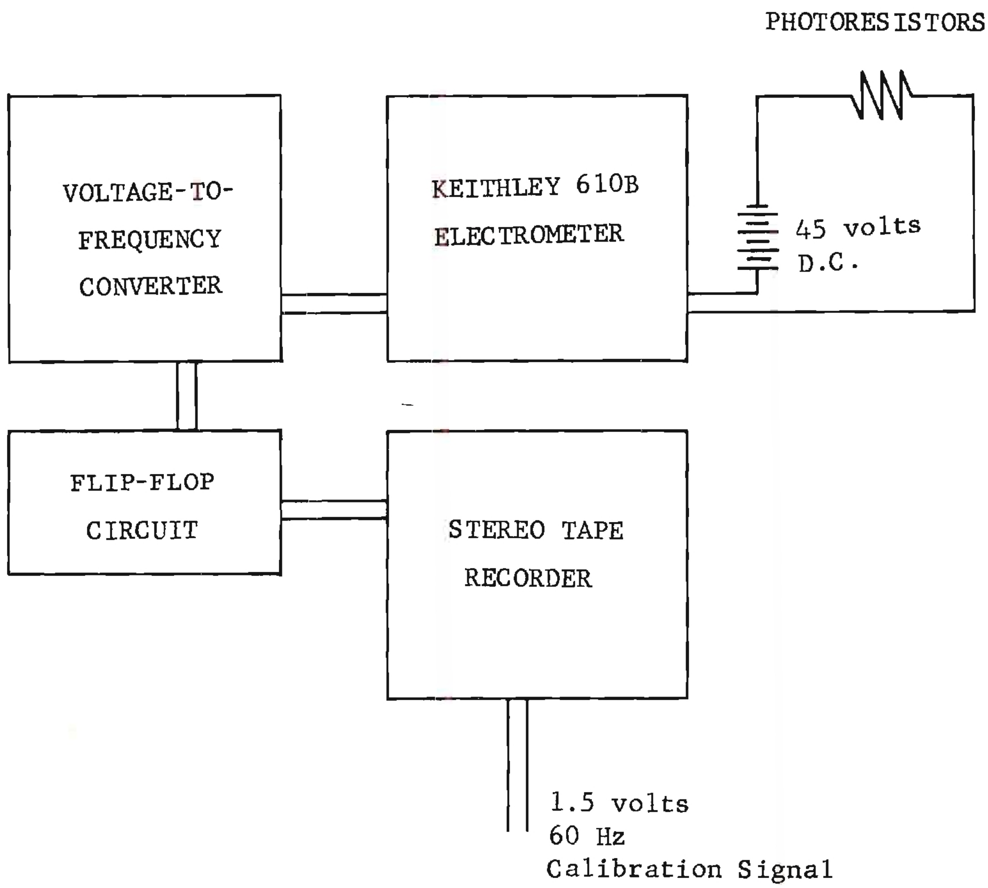


Fig. 3. Schematic Diagram of Electronics for Recording the Spectrum as a Frequency-Modulated Signal.

The output of the voltage-to-frequency converter consisted of a series of "spikes" about 2 μsec in width. The frequency with which the spikes are generated is a nearly linear function of the applied voltage. Since it is difficult for an inexpensive tape recorder to detect a signal with so narrow a half-width, the signal was fed into a flip-flop circuit to be converted into a square wave (with half the original frequency). This signal was recorded at 1-7/8 inches per second on 1/4 inch magnetic tape using one track of a 4-track stereo tape recorder.

The other track of the stereo tape recorder was used to record a stepped-down 60 Hz line signal. The 60 Hz signal was thereafter used to trigger the analog-to-digital converter, controlling its sampling rate. In this way, it was possible to compensate for random variations in the speed of the tape drive as well as stretching of the magnetic tape. Since the scanning densitometer was driven by a synchronous motor, this technique also compensated for variations in the scanning rate due to small fluctuations in the frequency of the line current.

The FM signal corresponding to the spectroscopic data was demodulated at the Rich Electronic Computer Center (RECC) using an Ampex SP-300 FM/AM tape recorder. The demodulated (DC) signal was adjusted to fall within a range of $\pm$ 1 volt and was used as input to a Radiation, Inc. Model 5020 analog-to-digital system.

The RECC analog-to-digital system has seven analog input channels which may be sampled in any order. Sampling may be triggered either by an internal clock or by an external clock. If an external clock is used, the system enables the user to generate up to seven sampling signals per clock pulse.

As mentioned above, a 60 Hz signal was used in this work to control the rate of sampling. In order to make the format of the digital magnetic tape produced by the analog-to-digital system conform to the normal input specifications of the Univac 1108, three channels were sampled per clock pulse: two channels without input, which entered zeros on the digital tape, and one channel with the desired analog signal.

The digital data were blocked in units of 513 Univac words (1001 octal); the first word specified the block number on the tape (a running index), and the remaining 512 words were data.

A variety of programs were written to process the digital data using a Univac 1108 computer equipped with a Calcomp plotter. These are described in detail in Appendix I. The usual sequence of operations was the following: (1) Scan the digital tape and plot the observed plate density as a function of plate position (1 mm of the photographic plate per inch of plot). (2) Expand the scale of the portion of the plate containing the iron calibration lines (1 mm of the plate per 10 inches of plot); the relative positions of the calibration lines on the digital tape could be determined very accurately by using this scale expansion technique and plotting both the spectrum and its first derivative. (3) Fit the vacuum wavelengths of the calibration lines to a quadratic or cubic equation in their relative position on the digital tape. (4) Plot the observed spectrum on a scale that is linear in frequency (either 1 cm^{-1} or 10 cm^{-1} per inch; when the former scale was used, the first derivative of the spectrum was also plotted).

Unblended lines of the high-resolution spectra could be reproduced to within .02 cm^{-1} using this technique; i.e., spectra from different photographic plates (and perhaps different dispersion) could be calibrated in this way, and the frequency of corresponding isolated lines would differ by no more than .02 cm^{-1}.

98 percent O^{18}-enriched oxygen gas was obtained from Miles Laboratories, and sulfur dioxide was prepared according to the method of Lichtin, et al. (23). Elemental sulfur was heated for four days at 250° with O_2^{18} in a reaction vessel filled with glass wool. An amount of sulfur slightly in excess of the stoichiometric amount was used to inhibit formation of SO_3. The entire reaction vessel was wrapped with electric heating tape and insulated to prevent condensation of sulfur at a cold spot in the vessel. The temperature was estimated by extrapolating temperature as a function of Variac voltage.

In light of conflicting reports that SO_2^{18} might exchange with Pyrex, the reaction system and sample cell were heated under vacuum to outgas any adsorbed water. All gas transfers were accomplished using break seals, and the iron rods used to break the seals were encapsulated in glass to minimize the adsorption of water. With these precautions, the SO_2^{18} was not observed to exchange with the cell over a period of several months, contrary to previous reports (23).

SO_2^{16} spectra were obtained using Matheson commercial grade SO_2 without further purification. Samples were maintained at -78°C by packing the absorption cells with dry ice. Dry air was continuously blown on the cell windows during each experiment to prevent condensation of moisture. Pressure in the cells were determined by the vapor pressure of sulfur dioxide (8 torr at -78°C).

CHAPTER III

PRELIMINARY OBSERVATIONS

The low-resolution absorption and magnetic rotation spectra of SO_2^{16} are reproduced in Figure 4. The region of greatest interest in magnetic rotation extends from 2900Å to about 3130Å; these limits correspond to the intense features of the absorption spectrum designated A, B, C ... by Clements. These features begin at least 2000 cm^{-1} above the system origin, as reported by Metropolis.

The relative intensities of bands in the magnetic rotation spectrum (MRS) are similar to those of the absorption spectrum, implying that the magnetic field effect is a property of the band system as a whole rather than a property of isolated transitions. That is, the magnetic properties of the excited state are fairly uniformly distributed among rovibronic levels. This is in contrast to that of molecules such as formaldehyde which exhibit a MRS for a singlet-singlet transition due to sharp perturbations of isolated lines by a nearby triplet system. In such spectra, the structure of the MRS bears little or no resemblance to the absorption spectrum.

A magnetic rotation spectrum may arise in three ways (26): the ground state may have a permanent magnetic moment; the excited state may have a permanent magnetic moment; or one of these states may acquire a magnetic moment from field-induced mixing with another state. Since there is no anomalously large magnetic moment associated with the ground vibronic state, as indicated by Zeeman studies of the microwave

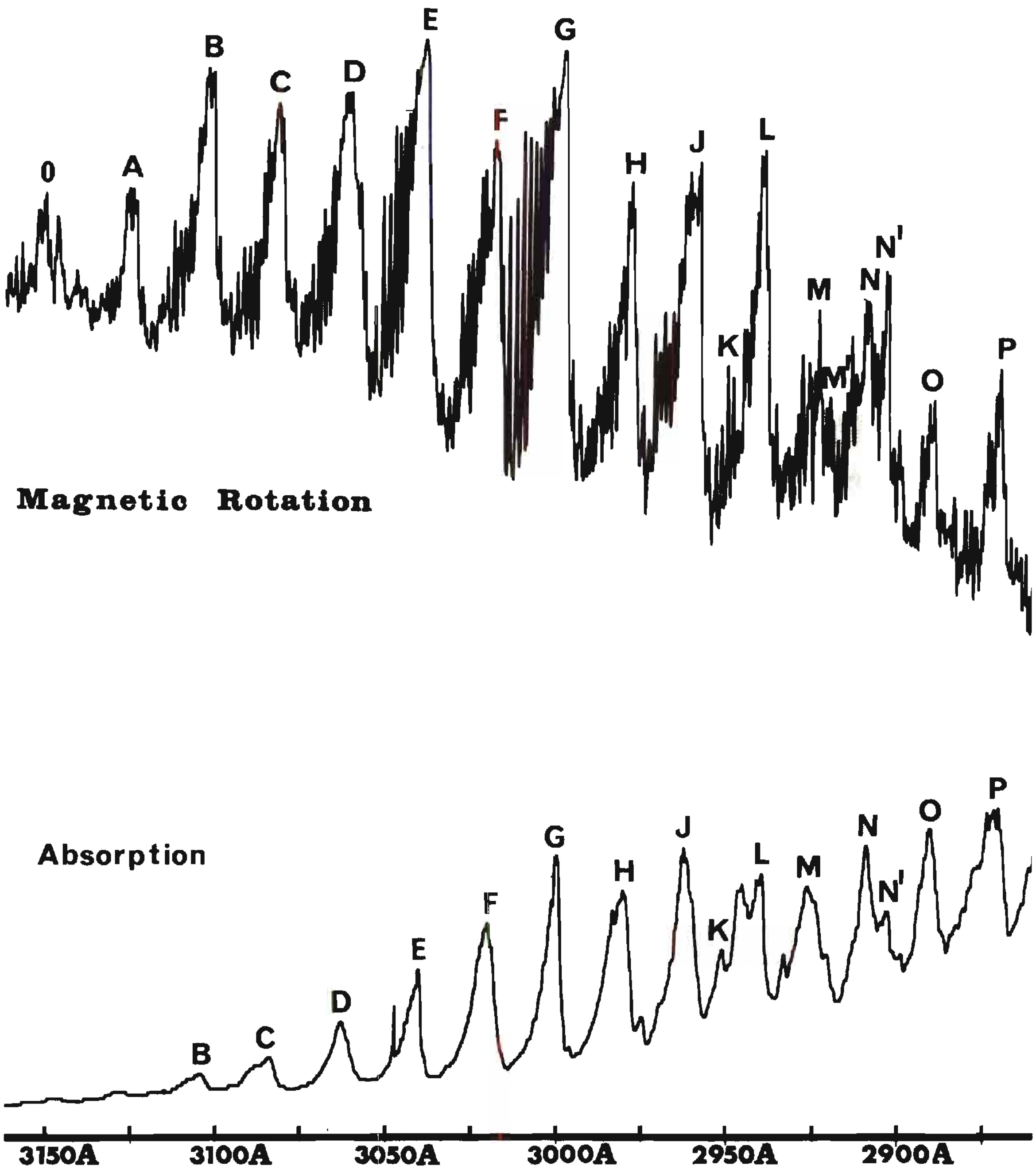


Fig. 4. Low-Resolution Absorption and Magnetic Rotation Spectra of SO_2^{16}.

spectrum (25), the MRS must arise from properties of the excited electronic state.

The excited state must, since it is a singlet state (24) acquire a magnetic moment through either zero-field or field-induced mixing with another electronic state. There are three obvious candidates for the perturbing state: the $^3B_1$ state (through vibronically induced spin-orbit coupling); the $^3B_2$ and $^3A_2$ states, which have not been observed but which are anticipated to fall in this region of the spectrum (27) (through spin-orbit coupling); and the ground state (through Renner-Teller rovibronic coupling).

In part to determine the nature of the perturbing state and in part to test the reliability of calculated rotational constants, the magnetic rotation spectrum of the O^{18}-enriched species was observed. The magnetic rotation spectra of the two species are essentially similar, as may be seen by comparing the low-resolution spectra reproduced in Figure 5. This similarity is further confirmation that the magnetic field effect is uniformly distributed over the band system and is not due to sharp, isolated perturbations. Thus, the magnetic properties of the excited state cannot be ascribed to accidental degeneracy with the widely spaced levels of another excited state, but must instead be due to mixing with a quasi-continuum of levels such as the vibrationally excited levels of the ground electronic state.

Thus it appears that rovibronic mixing of the excited electronic state with the ground electronic state, in addition to being responsible for the anomalous fluorescence lifetime, is also responsible for the magnetic rotation spectrum.

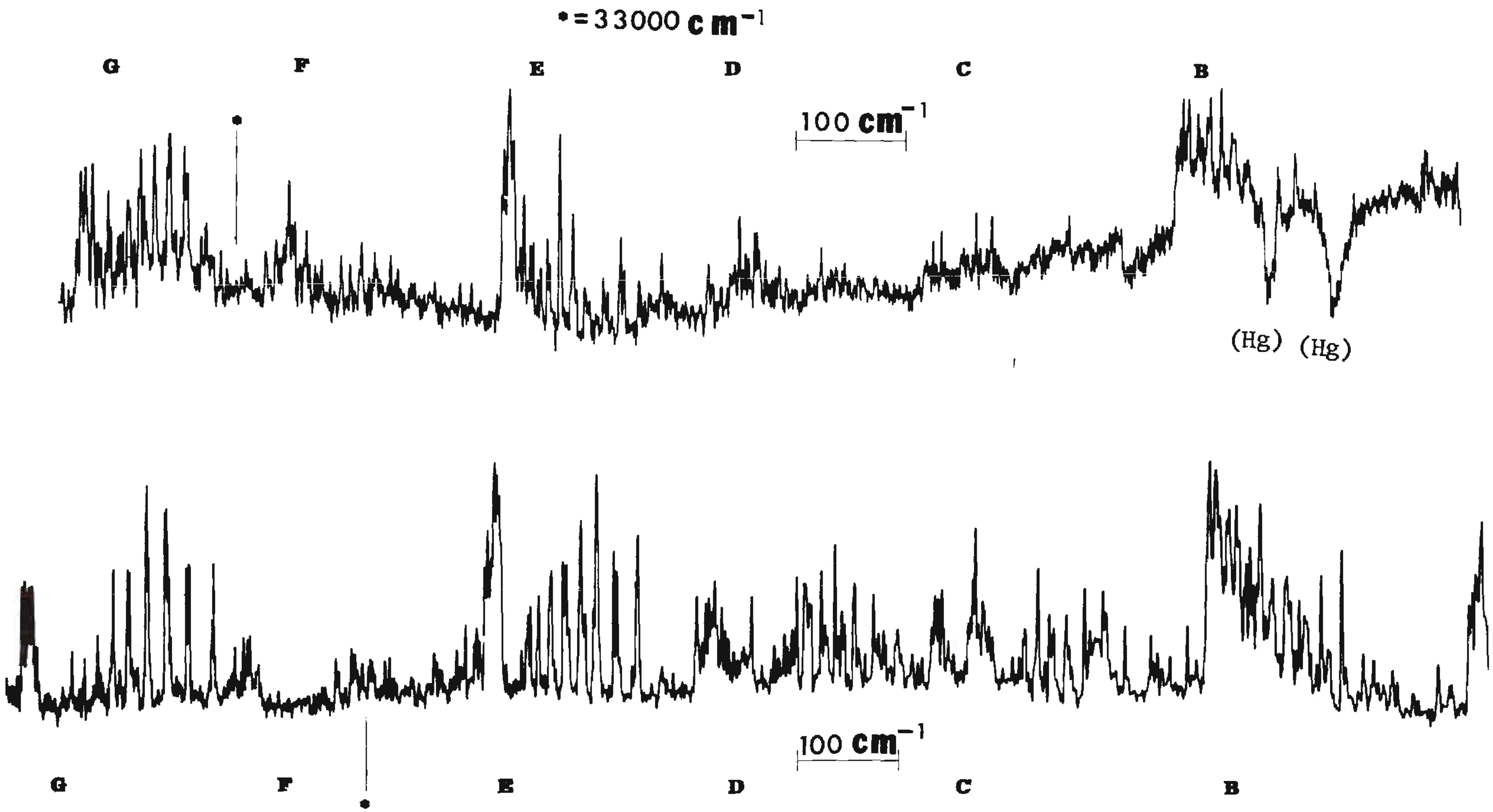


Fig. 5. Low-Resolution Magnetic Rotation Spectra of SO_2^{16} (Lower) and SO_2^{18} (Upper).

The high-resolution absorption spectrum of a portion of the E band of SO_2^{18} is reproduced in Figure 6. The corresponding magnetic rotation spectrum is reproduced in Figure 7. Since the sub-band structure is much more obvious in the MRS than in the absorption spectrum, our efforts have been directed toward interpreting the rotational fine structure of the MRS.

Assuming that the prolate symmetric rotor quantum numbers J and K are appropriate to describe the excited state, the coarse structure of the bands we have studied indicates that the most prominent transitions are to be ascribed to the selection rules $\Delta J = \Delta K = \pm 1$ or ± 2. As mentioned above, this analysis is predicated on the assumption that the magnetic effect depends solely upon properties of the excited state rovibronic levels; i.e., the widely spaced branches to the red and the densely packed branches to the violet arising from transitions to the same excited state will be of comparable intensity.

Based on the accurately known (35) rotational constants of the ground state, combination relations were used to relate the fine structure of the red-degraded sub-bands with that of the sub-bands clustered at the violet end of each band. It was _not_ possible to reproduce the observed band structure assuming that $\Delta K = \pm 1$ and all values of K' are present for any given band. Combination relations _could_, however, be reproduced for all observed sub-bands assuming $\Delta K = \pm 1$ and _only_ even or odd K' are present for any one of the vibronic bands studied. Excited state term values could then be fitted to a symmetric top energy formula with reasonable accuracy for low values of K'. The fit becomes increasingly poorer as K' approaches v_2'; this trend is not surprising, as explained in chapter IV.

* Fe emission

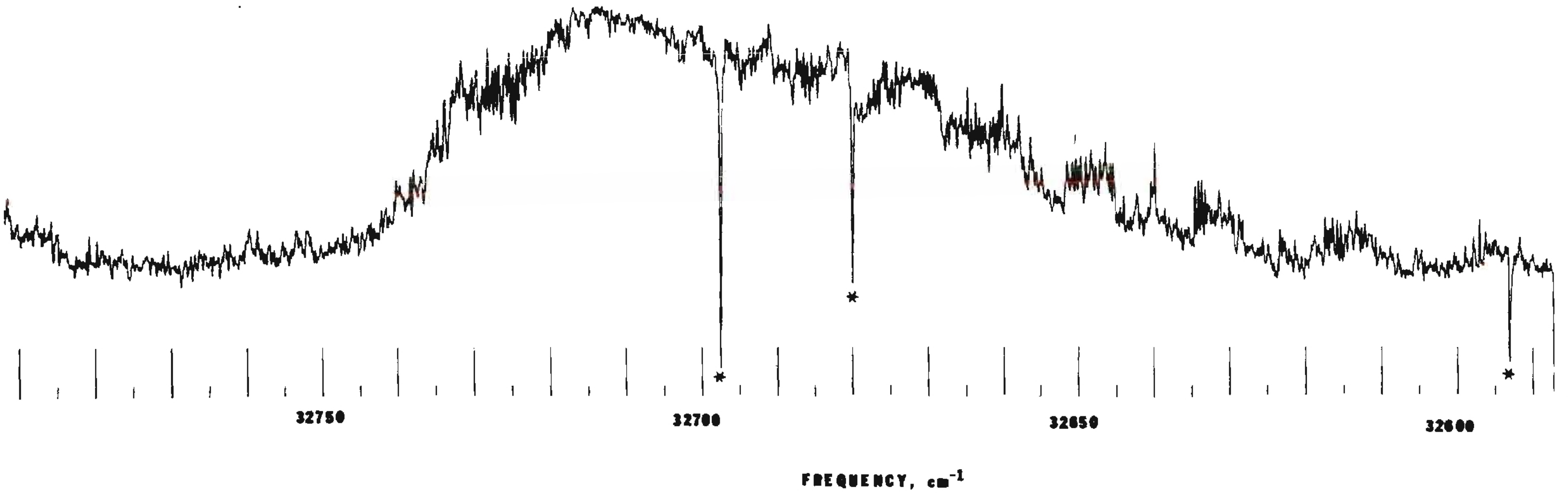


Fig. 6. High-Resolution Absorption Spectrum of the SO_2^{18} E Band.

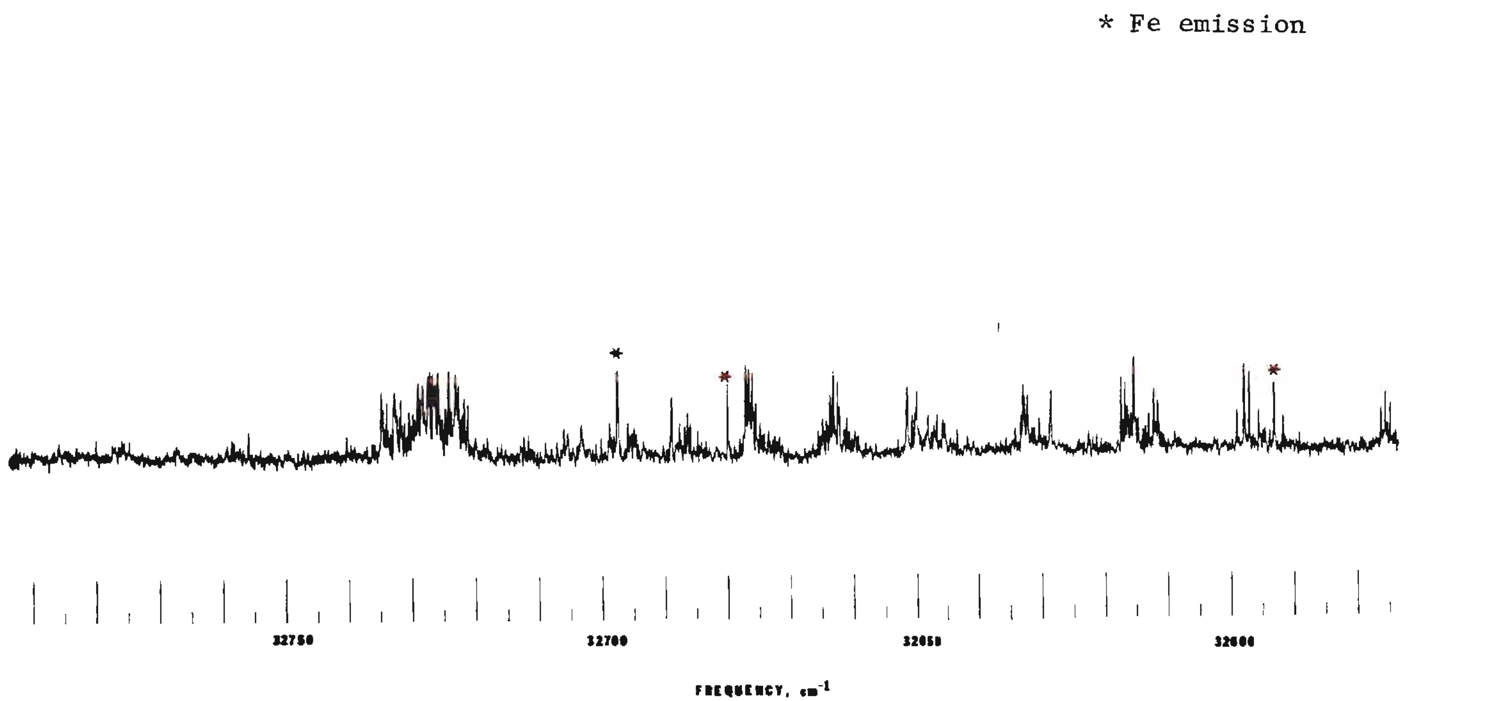


Fig. 7. High-Resolution Magnetic Rotation Spectrum of the SO_2^{18} E Band.

Although the observed band structures could be reproduced qualitatively assuming all values of K' present and $\Delta K = \pm 2$, this hypothesis was rejected for two reasons. First, combination relations for sub-bands corresponding to high values of K' could not be reproduced satisfactorily. For $K' \geq 10$, it became necessary to assume that, for the leading line of a sub-band, $J'=2K'$. There is no obvious theoretical justification for such an assumption. And second, the quantitative fit of the excited state term values to a simple symmetric top energy formula was much poorer.

The appearance of only even or odd values of K' within a given vibronic band implies that either the molecule is linear in its excited state, or the energies of the rovibronic states under consideration are less sensitive to a barrier to linearity than to anharmonicity associated with large values of the bending co-ordinate. If the bending potential function is approximated by a convenient two-dimensional, isotropic, harmonic potential function, all vibronic levels associated with a given value of the bending quantum number, v_2', will be degenerate. A perturbation of the harmonic function by a barrier to linearity leads to a <u>lowering</u> of energy for increasing magnitude of the vibrational angular momentum, ℓ; perturbation of the harmonic function by a term quartic or higher in the bending co-ordinate may lead to a <u>raising or lowering</u> of vibronic energy with increasing ℓ, depending on the sign of the term. Since energy increases with increasing angular momentum about the figure axis, there is no immediate necessity of considering a nonlinear equilibrium configuration. The introduction of Renner-Teller coupling further complicates the dependence of energy on vibronic angular momentum, as discussed in chapter IV.

The selection rule $\Delta K = \pm 1$ implies that the excited state has A_1 or B_1 symmetry, since the transition moment must be polarized perpendicular to the figure axis. The only electronic state of A_1 symmetry likely to appear in this region of the spectrum is the ... $(b_1)^2$ A_1 state obtained from the ... $(\pi^*)^2$ $^1\Sigma_g^+$ linear conformation of the molecule. Since this represents a two electron promotion from the ground state, it is unlikely that the observed transition is to the A_1 electronic state. Moreover, there is no obvious mechanism for the excited $^1A_1$ $(^1\Sigma_g^+)$ electronic state to acquire a magnetic moment through mixing with the ground state. An assignment of the excited state as having $^1B_1$ symmetry appears, then, to be the most plausible alternative.

CHAPTER IV

MODEL OF THE EXCITED STATE

Most molecular calculations are carried out within the framework of the Born-Oppenheimer approximation; that is, the Hamiltonian is separated into an electronic and a nuclear part:

$$H^o \approx H^o_e + H^o_n \tag{1}$$

and the rovibronic wavefunction is approximated by a product function (28)

$$\Psi_{evr} \approx \Psi_e \Psi_n \tag{2}$$

This approximation is good only insofar as the energy of the nuclear motions is small compared with the energy separating electronic states. When the energy associated with nuclear motions is not negligible compared with the energy difference between electronic states, the two eigenvalue problems become coupled, and cross terms in the Hamiltonian can no longer be ignored:

$$H_{tot} = H^o + H^1_{en} \tag{3}$$

$$\Psi_n H^o_e \Psi_e + H^1_{en} \Psi_e \Psi_n = E_e \Psi_e \Psi_n \tag{4}$$

$$\Psi_e H^o_n \Psi_n + H^1_{en} \Psi_e \Psi_n = E_n \Psi_e \Psi_n \tag{5}$$

This coupling is of quite general occurrence in eigenvalue problems when off-diagonal matrix elements (here, H^1_{en}) are of magnitude comparable to the diagonal elements (the eigenvalues of the zeroth-order Hamiltonian).

In diatomic molecules, the Born-Oppenheimer approximation breaks down slightly due to the Λ-type doubling of rotational levels, for example. The coupling is necessarily small, since angular momenta which are perpendicular to one another are being coupled. The vibrations of a diatomic molecule are, of course, of Σ symmetry, and there is no term in the total Hamiltonian which can couple them directly to the electronic orbital angular momentum.

In a triatomic molecule, on the other hand, the bending vibration can couple directly to the electronic angular momentum of a degenerate electronic state. Choosing a zeroth-order separation of the rovibrational Hamiltonian into a stretching term, a linear rotor term, and a two-dimensional bending term (29), the vibrational eigenfunctions will be of the form

$$\Psi_n = \Psi_{vib}(Q_1,Q_3)\,\Psi_{rot}(J_x,J_y)R(Q_2)\,e^{i\ell\varphi} \tag{6}$$

Here the factor of interest is

$$R(Q_2)\,e^{i\ell\varphi}$$

which consists of a "radial" factor in the amplitude of the bending co-ordinate, Q_2, and a "vibrational angular momentum" factor, $e^{i\ell\varphi}$. Throughout this work, unless otherwise noted, Q_2 will be approximated by a rectilinear displacement, x, perpendicular to the figure axis of the prolate symmetric top.

The vibrational angular momentum will be parallel to the electronic orbital angular momentum and will couple to it by cross terms in the Hamiltonian of the form

$$\frac{h^2}{8\pi^2 m}\frac{\partial}{\partial\varphi}\ \frac{\partial}{\partial\varphi_e}$$

Pople and Longuet-Higgins (30) have shown that the vibronic levels of a triatomic molecule derived from a degenerate electronic state may be represented by perturbing a product basis set of the form $|v_2, \ell\rangle|\Lambda\rangle$ with a perturbing Hamiltonian of the form

$$\mathbf{H}' = V_o(x) + V_1(x)\cos\alpha + V_2(x)\cos 2\alpha + \ldots \tag{7}$$

Here $|v_2, \ell\rangle$ are solutions of the vibrational Schrodinger equation

$$-\frac{h^2}{8\pi^2 m}\nabla^2\Psi_b(x,\varphi) + V_o(x)\Psi_b(x,\varphi) = E\,\Psi_b(x,\varphi) \tag{8}$$

$U_o(x)$ is the potential function of a hypothetical unperturbed degenerate electronic state, α is the difference between the co-ordinates conjugate to the electronic and nuclear angular momenta about the figure axis, and V_o and V_i are functions only of x.

Since it is not the purpose here to perform exact calculations of the Renner effect in sulfur dioxide, only the qualitative features of the applications of this type of perturbation treatment will be presented.

The Renner effect may cause a splitting of the components of a few hundred reciprocal centimeters, as in NCN (31) or several thousand, as in SO_2, depending on the details of the molecular orbitals involved. Of course, when the splitting is very large, it may become convenient to make a different Born-Oppenheimer separation and treat the two components as different electronic states. Although the two formalisms will ultimately yield the same results if calculations are carried out exactly, it is by no means obvious that calculations will be the same in any convenient intermediate approximation.

Renner's original paper (45) considered only the splitting of a linear Π electronic state by a perturbing Hamiltonian quadratic in the molecular bending co-ordinate. Since this treatment implies that the potential functions in x generated by both components of the electronic state are harmonic, and will have minima in the linear configuration, it is useful only in the "weak coupling" case. In stronger coupling cases, higher order terms become important and one or both of the potential functions will have minima corresponding to a nonlinear equilibrium geometry. Renner's conclusions were that the energy of a Π vibronic state which is not degenerate in the zeroth order will be given by

$$G(v_2K) = \omega_2(v_2+1) - \epsilon^2K(K+1) \tag{8}$$

where ϵ is a dimensionless perturbation parameter varying between -1 and 1; for a pair of degenerate Σ vibronic states

$$G\ (v_2,0) = \omega_2\sqrt{1 \pm \epsilon}\ (v_2+1); \tag{9}$$

and a pair of degenerate Π, Δ, ... vibronic states will be split in the first order according to the formula

$$G\,(v_2,K) = \omega_2(1-\frac{1}{8}\epsilon^2)(v_2+1) \pm \frac{1}{2}\omega_2\epsilon\sqrt{(v_2+1)^2-K^2} \qquad (10)$$

Σ vibronic states are characterized by the additional symmetry operation of reflection of the total vibronic wavefunction in the molecular plane, and are denoted Σ^+ and Σ^-. A set of vibronic wavefunctions of Σ^+ symmetry will define the bending potential function of one component of the electronic state, while the potential function of the other component will be defined by the vibronic functions of Σ^- symmetry. The Σ^+ and Σ^- vibronic states will have no nonvanishing term of the Hamiltonian operator connecting them, and they will cross each other as ϵ becomes large.

For Π, Δ,... vibronic states, the situation is more complex. States "belonging" in a first approximation to the upper or lower electronic component will have nonvanishing matrix elements of the perturbing Renner Hamiltonian connecting them, and will undergo strong avoided crossings (Figure 8).

Renner's formulas have been useful in describing the Π electronic states of C_3(32), CCN(33), CNC(34), NCN(31), NCO, N_2O^+, N_3, BO_2, and other isovalent species (36). In these molecules, both components of the Π electronic states being considered have linear equilibrium configurations.

If the bending potential function described by one or both of the components of the degenerate electronic state has a maximum in the

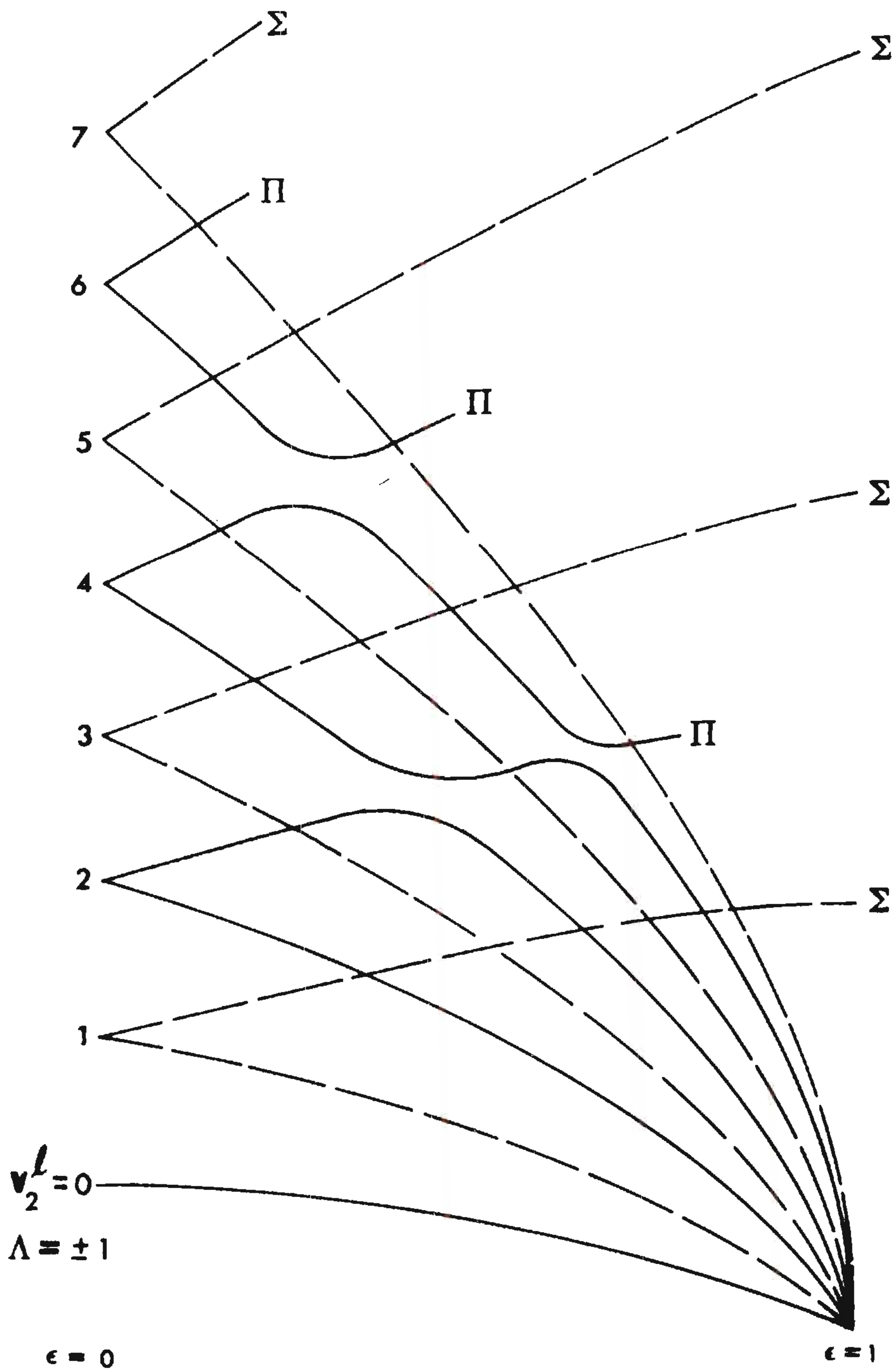


Fig. 8. Energy of the Σ and Π Vibronic States of a Linear Molecule as a Function of Renner-Teller Coupling [After Renner (45)].

linear configuration of the molecule (i.e., a bent equilibrium configuration), the treatment given by Renner is no longer appropriate.

Pople and Lonquet-Higgens (30) have considered the case of a harmonic potential perturbed by a term in the Hamiltonian of the form

$$H' = -\tfrac{1}{2}fx^2 + \tfrac{1}{2}(g+h)x^4 + \left[\tfrac{1}{2}fx^2 - \tfrac{1}{2}(g-h)x^4\right]\left[2\cos 2\alpha\right]$$

and applied their results to the upper component of the $^2\Pi$ state of NH_2. They found that the term values of the upper state were given by

$$G(v_2, K) = \omega_2 \left\{ (v_2+1) - \tfrac{1}{2}f\left[v_2+1 - \sqrt{(v_2+1)^2 - K^2}\right] + \tfrac{1}{4}(g+h)\left[3(v_2+1)^2 - K^2\right] - 3/4(g-h)(v_2+1)\sqrt{(v_2+1)^2 - K^2} \right\} \quad (11)$$

The term values for the lower level could not be computed by this technique, since the perturbing term in the Hamiltonian was not chosen to reproduce the potential function of the ground state accurately.

Dixon (37), also attempting to interpret the splitting of the $^2\Pi$ electronic state of NH_2, perturbed a harmonic oscillator basis set with a combination of quadratic and Gaussian functions of x. This technique allows both the upper and lower potential functions to have bent equilibrium configurations. In this approximation, the bending potential function of the ground state $^2B_1$ component may be represented well by the perturbing Hamiltonian; the term values of the upper component may be reproduced more closely than in the treatment of Pople and Longuet-Higgens; and the "avoided crossings" of non-Σ vibronic states may be predicted to a fair approximation. (In the approximation that the upper and lower components represent different Born-Oppenheimer states, these avoided crossings may be interpreted as rovibronic mixing of the two states.) Unfortunately, the numerical perturbation treatment of Dixon yields no simple analytic expression for the term values of the two states.

The splitting of the $^2\Delta$ state of CCN has been studied by Merer and Travis (33). These authors used a pure quartic perturbing Hamiltonian:

$$H' = \eta x^4 \cos 4\alpha \tag{12}$$

The quadratic term in x in the perturbing Hamiltonian is identically zero for a Δ state; in general, the first nonvanishing term in the α -dependent part of the Hamiltonian will be (30)

$$H'_o = \gamma x^{2|\Lambda|} \cos(2|\Lambda|\alpha) \tag{13}$$

Since a quadratic potential function perturbed by a quartic term is inadequate to describe a Δ state in which one or more component has a nonlinear equilibrium configuration, the formulas of Merer and Travis should be expected to be appropriate only to calculate the term values of the weak coupling case. The molecules to which their treatment has been applied successfully both have splittings of a few hundred reciprocal centimeters or about the energy of a vibrational frequency.

The term values of the Δ electronic state, like those of the Π state, are classified according to whether the state is a vibronically nondegenerate state or one of a pair of vibronically degenerate states. The energies of a pair of the latter will be given by

$$G^{\pm}(v_2,K) = \omega_2(v_2+1) \pm \tfrac{1}{2}\left\{64K^2g^2 + 36\eta^2\left[v_2^2-K^2\right]\left[(v_2+2)^2-K^2\right]\right\}^{\frac{1}{2}}$$

$$-\frac{\eta^2}{\omega_2}(v_2+1)\left[17(v_2+2)+3K^2\right] + g(K^2+4)$$

$$\pm 4\frac{\eta^2}{\omega_2}g(v_2+1)K^2\frac{\left[17v_2(v_2+2) - 15K^2 + 72\right]}{\left\{64K^2g^2+36\eta^2\left[v_2^2-K^2\right]\left[(v_2+2)^2-K^2\right]\right\}^{1/2}} \tag{14}$$

while that of the former will be given by

$$G(v_2,K = v_2) = \omega_2(v_2+1) - \frac{\eta^2}{\omega_2}K(K+1)(K+2)(K+35) + g(K-2)^2 \tag{15}$$

and

$$G(v_2,K = v_2+2) = \omega_2(v_2+1) - \frac{\eta^2}{\omega_2}(K-1)K(K+1)(K+2) + g(K-2)^2 \tag{16}$$

(We are ignoring any term due to electron spin.)

As with the case of a Π electronic state, only Σ^+ and Σ^- vibronic states do not interact with one another; the Π, Δ,... vibronic states associated in the first order with a given component of the degenerate state will undergo strong avoided crossings with vibronic states of the same symmetry but associated with the other component.

A given degenerate pair of vibronic states will, in general, be split in the first order as

$$\psi^{\pm}(v_2,K) = |v_2,K\ \ell = K-2,\ \Lambda = 2\rangle \pm |v_2,K,\ \ell = K+2,\ \Lambda = -2\rangle \qquad (17)$$

and the expectation value for Λ will, to a first approximation, be zero. In an instance of an avoided crossing, however, a wavefunction of the form $\psi^{+}(v_2,K)$ will mix with a wavefunction of the form $\psi^{-}(v_2',K)$; the resulting (unnormalized) wavefunctions will have the form

$$\psi^{+'}(v_2,K) = \psi^{+}(v_2,K) + \delta\psi^{-}(v_2',K) \qquad (18)$$

$$\psi^{-'}(v_2',K) = \psi^{-}(v_2',K) - \delta\psi^{+}(v_2,K) \qquad (19)$$

$\psi^{+'}$ and $\psi^{-'}$ will both, then attain nonvanishing expectation values for Λ (and a consequent magnetic moment) due to vibronic mixing.

A rigorous treatment of a Δ state split by a strong Renner effect (on the order of several thousand cm^{-1}) has not been given. A qualitative treatment of the effect has been given by Merer and Travis (39) in their discussion of the spectra of HCCl and DCCl. In the 5500-8200Å system, which is assigned as $^1A'(^1\Delta) \leftarrow {}^1A''(^1\Delta)$, the rotational structure corresponding to sub-bands with $K' > 0$ appears quite complex. This observation is interpreted as due to rovibronic mixing of the two components.

In light of recent theoretical developments dealing with the vibrational and rotational energies of triatomic molecules, the most reasonable way to approach the problem seems to be that of choosing a zeroth order Hamiltonian consisting of an isotropic two-dimensional harmonic potential function perturbed by a Gaussian or Lorentzian hump; and a kinetic energy operator which accounts for the curvilinear coordinates described by Hougen, Bunker, and Johns (40) and Bunker and Stone (41). The basis set described by this Hamiltonian could then be perturbed numerically by the perturbing Hamiltonian used by Merer and Travis. Such a calculation is, however, beyond the scope of this work. The correlation of states will be slightly different in this treatment than in the usual one (see Figure 9), and the quenching of Λ will no longer be complete for states with $K > 0$ (see Figure 10).

Since the observations of Chapter III indicate that the splitting of the two components is on the order of 25-30,000 cm^{-1}, we will assume that a strong coupling case is appropriate to describe the $^1\Delta_g$ state of SO_2; and the lower and upper components will be referred to, for the sake of convenience, as $^1A_1$ and $^1B_1$ electronic states. Furthermore, since the "vibrational angular momentum" of the linear or nearly linear $^1B_1$ state is in reality the vibronic angular momentum $(\Lambda + \ell)$ of one component of the $^1\Delta_g$ state, it will be denoted as K rather than ℓ.

In this approximation, the vibronic energy levels of the $^1B_1$ component bear a formal resemblance to those of a linear molecule in a Σ_g^- electronic state. That is,

$$K = v_2', \; v_2'-2, \ldots 1 \text{ or } 0$$

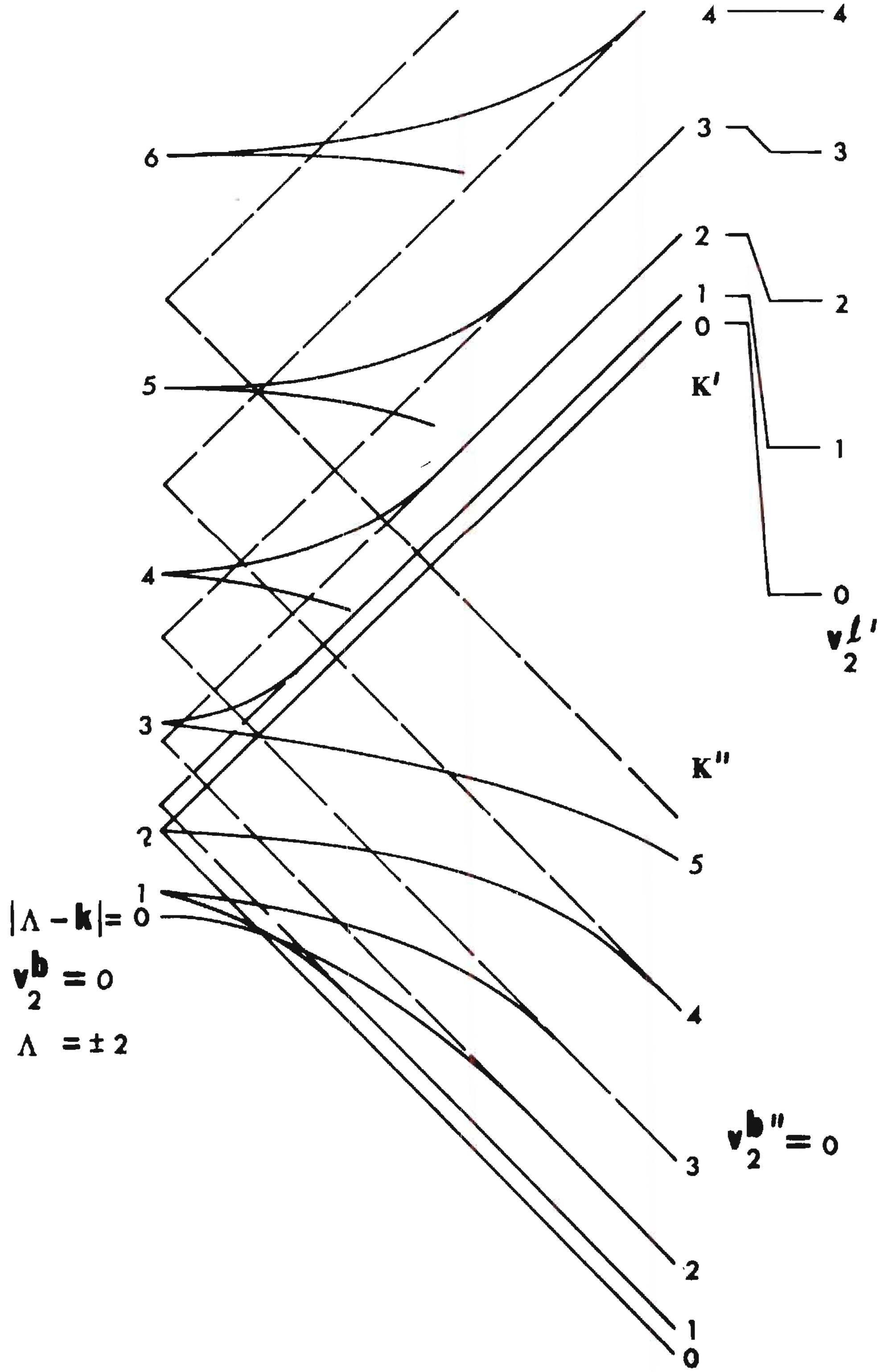


Fig. 9. Energy of a Bent Molecule as a Function of Renner-Teller Coupling.

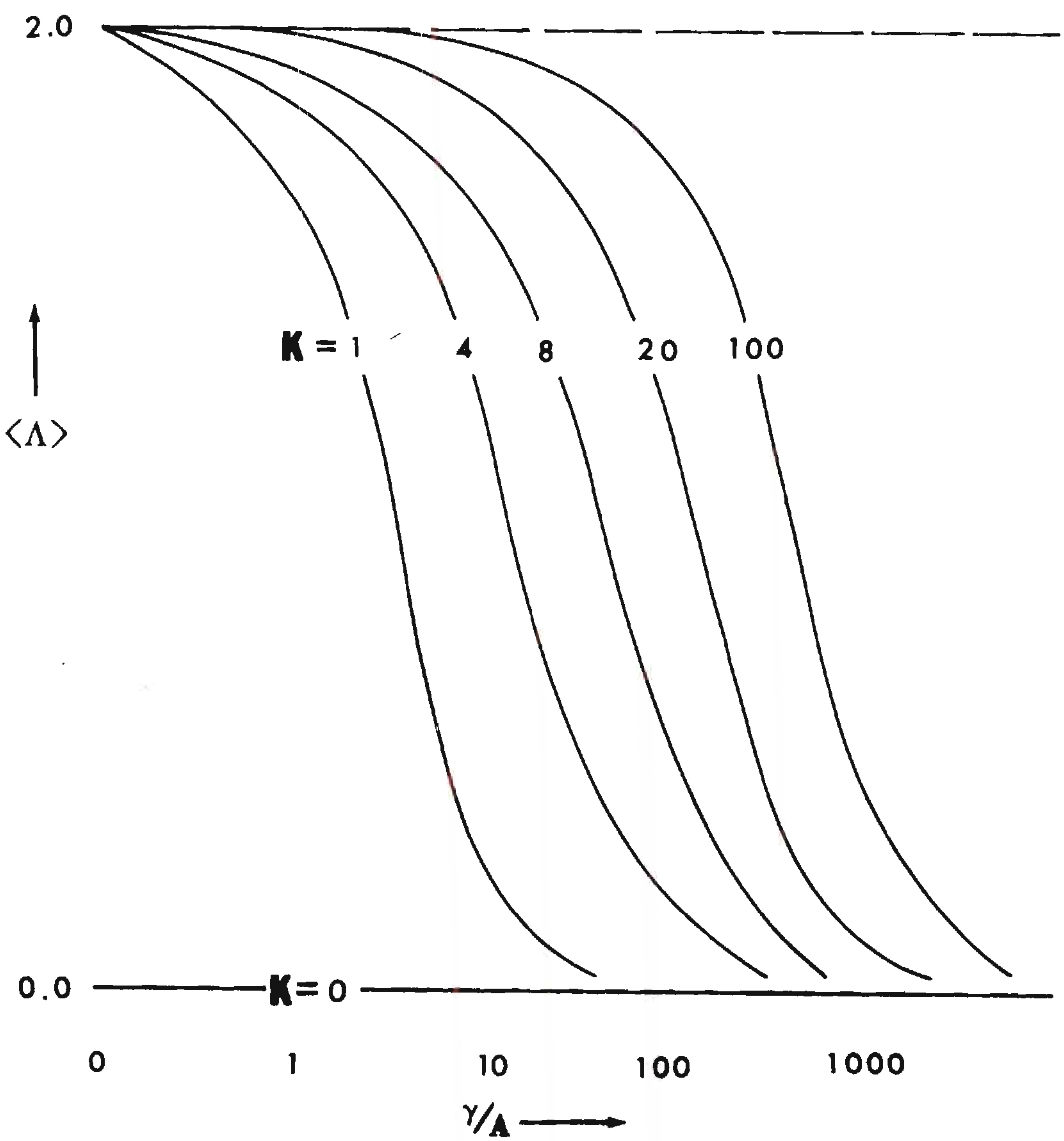


Fig. 10. Quenching of Electronic Orbital Angular Momentum as a Function of Renner-Teller Coupling.

The degeneracy of states with the same value of v_2 but different values of ℓ is removed in a Σ electronic state by anharmonic terms in the bending potential function. In the linear upper component of a degenerate electronic state, however, the vibronic term values are in general determined by the potential functions of both components; the manner in which the K-degeneracy is lifted will, therefore, bear no simple relationship to the potential function of the upper component.

This statement may be illustrated by expanding the energy formulas of Merer and Travis as a Taylor series in K and truncating the expansion with the term in K^2:

$$E = AK^2 + B\left[J(J+1)-K^2\right]$$

$$A = -\frac{8g^2-9\eta^2(v_2^2+2v_2+2)}{3\eta\, v_2(v_2^2+2)} - \frac{3\eta^2}{\omega_2}(v_2+1) + g$$

$$-\frac{\eta g}{\omega_2}\,\frac{(v_2+1)}{v_2(v_2+2)}\left[\frac{34}{3}v_2(v_2+2)-48\right] \qquad (20)$$

This formula will reproduce the original second-order perturbation formula to a good approximation for $K' << v_2'$, and, therefore, it is possible to employ a symmetric top formula for the term values of the excited state:

$$E(v_2,J,K) = G(v_2)+(A-B)K^2+BJ(J+1) \qquad (21)$$

The constant A will, however, be difficult to interpret, and in general will have a complicated dependence on v_2 and on isotopic substitution.

CHAPTER V

DETAILS OF THE ANALYSIS

Proceeding on the assumption that the strong features of each vibronic band are ^{p}P and ^{r}R branches, for the reasons indicated in Chapter III, detailed assignments of the rotational structure of each band were attempted. Progress was hampered by the presence of a background of weak lines with no obvious structure (see Figure 11). Presumably, this background is due either to intensity borrowing by high-energy levels of the ground electronic state or to weaker transitions to a nearby vibrational level of the excited electronic state. In general, it was not possible to distinguish the weak ^{p}R and ^{p}Q branches from this background, and no assignments could be based on these combination relations.

Moreover, since blending is so pronounced at the violet ends of these bands, there are many rotational assignments possible for each line based on combination relations of the ^{p}P and ^{r}R branches. The situation is further complicated by the self-absorption of the magnetic rotation spectrum (see Figure 12). As pressure of the sample is increased, the increase in intensity of the MRS due to increased rotation and ellipticity of the polarized light is compensated for by increased absorption by the sample. Thus, at high pressures, the intensity of the MRS will decrease with increasing pressure. Since the absorbing lines are not necessarily the same as those which give rise to magnetic

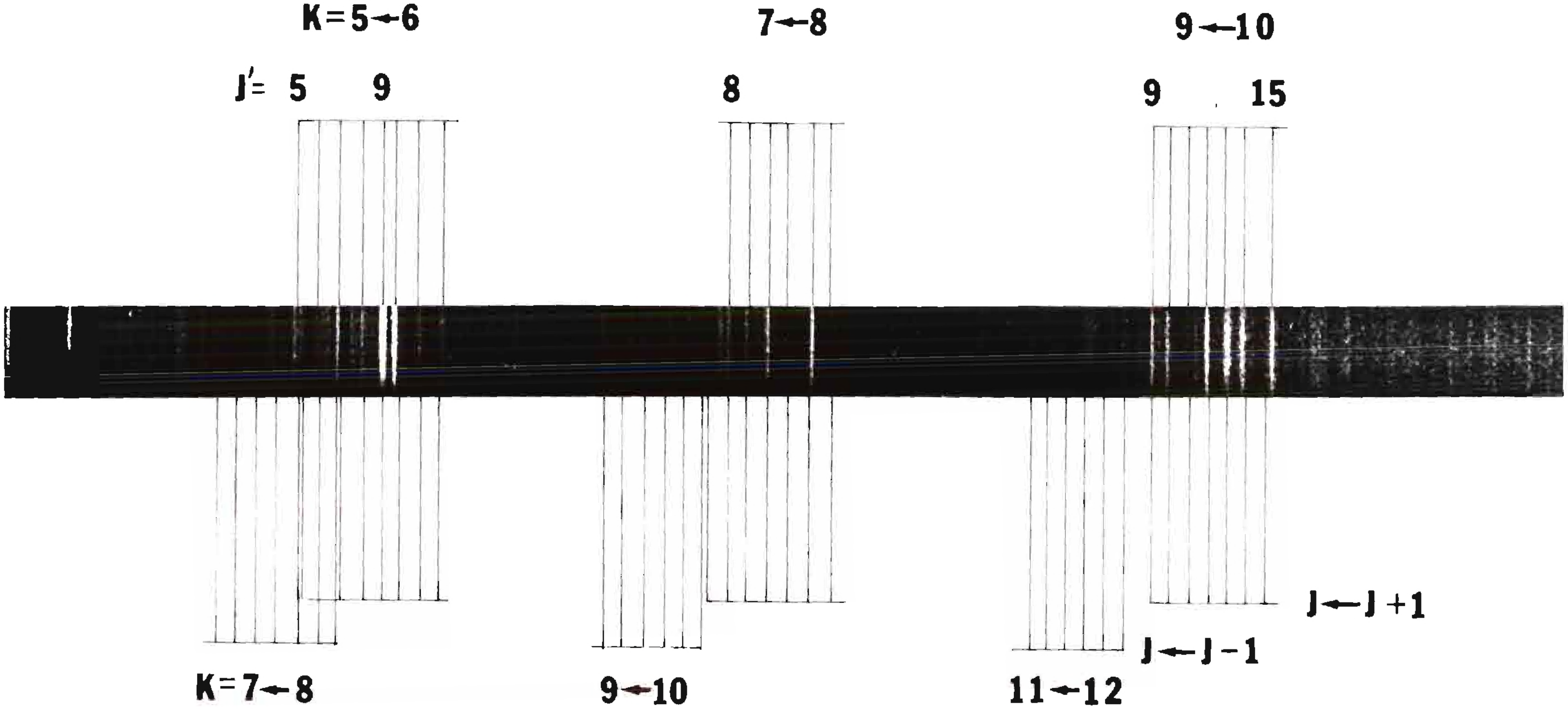


Fig. 11. Assigned (Upper) and Calculated (Lower) Rotational Structure of Part of the G Band of SO_2^{16}.

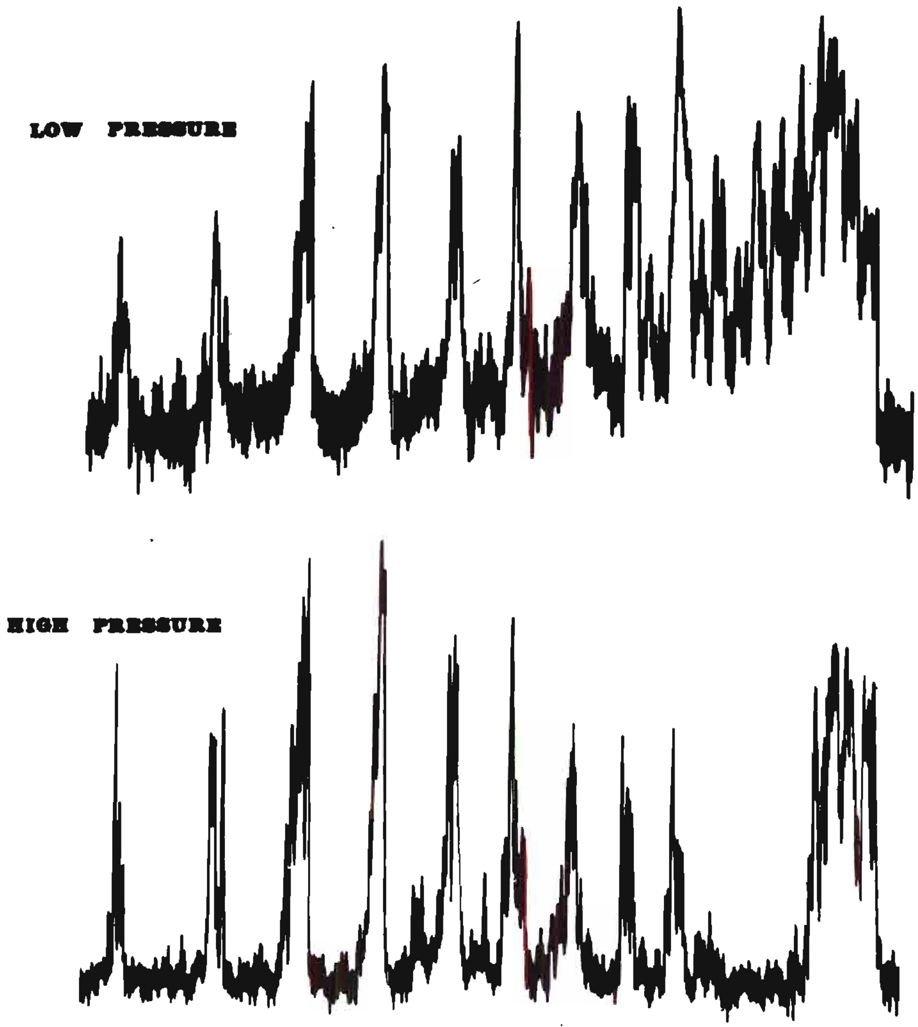


Fig. 12. Self-Absorption of the Magnetic Rotation Spectrum of SO_2^{16} in the G Band.

rotation (i.e., many lines are magnetically insensitive), this phenomenon will be of different importance for different regions of the spectrum. Thus, assignments of lines of the magnetic rotation spectra cannot be based on intensity.

A model for excited state term values was, therefore, employed at an early stage in this work. Trial assignments were entered from a time-sharing computer terminal for a few lines of a given band. The program then retrieved the ground state rotational term values from storage, computed the excited state term values based on the trial assignments, and calculated a least-squares fit of the excited state term values to the symmetric top formula described above. Output included the band origin, the computer rotational constants, the deviation of each assigned line from its calculated frequency, and, if requested, the calculated positions of other lines in the band. Details of the program may be found in Appendix I.

Using this technique, we were able to fit, within 0.1-0.2 cm^{-1} rms deviation, between 25 and 50 of the ^{P}P transitions and an equal number of ^{r}R transitions for each of ten bands, five of each isotopic species. We were then able to calculate the positions of lines in other branches and to account for many weaker lines in this way (see Figure 11).

The relatively large rms deviation (compared with the precision of our measurements) appears to be inherent in the model of a simple, unperturbed, symmetric rotor excited state. Comparing the sub-bands illustrated in Figure 11, it is apparent that, while some excited state energies are relatively unperturbed, many suffer from strong perturbations which we have no choice but to treat as random. For example, in the SO_2^{16} G band, ^PP transitions for K'=9 appear quite regular except for that corresponding to J'=11, which is anomalously weak. The ^PP branch for K'=7 is much more erratic, and the transition to J'=7 appears to be missing. The transitions to J'=9 and 10 for the ^PP branch with K'=5 are anomalously intense in magnetic rotation and are more closely spaced than other members of the sub-band. The transitions to J'=9 and 10 in the ^PP branch for K'=5 are anomalously intense in magnetic rotation and are more closely spaced than other members of this sub-band.

The band origins and rotational constants for the bands analyzed in this way are listed in Table 1. Some bands, notably the D band of both isotopic species, are exceedingly complex and have not yet yielded to analysis. We are unable at present to advance any reasonable explanation for this complexity.

The rotational constants, although varying only a few percent from band to band, appear to vary in an irregular manner that is difficult to interpret in terms of the molecular potential function. This difficulty arises in part from the difficulty in interpreting A' and in part from the lack of a reliable vibrational assignment for these bands.

The apparently random variation B' is especially disturbing, since it precludes any simple correction for the effects of large vibrational amplitude. This could, of course, be a reflection of the complexity of the potential function for the excited state bending co-ordinate. It is possible, however, that an uncertainty in the

Table 1. Band Origins and Rotational Constants.

Band	ν_0 SO_2^{16}	ν_0 SO_2^{18}	A SO_2^{16}	A SO_2^{18}	B SO_2^{16}	B SO_2^{18}
G	33325.7	33153.4	1.8492	1.7509	0.3214	0.2889
F	33098.4	32936.3	1.8214	1.7538	0.3212	0.2897
E	32865.9	32714.8	1.8344	1.7469	0.3225	0.2882
D						
C	32397.0		1.8786		0.3120	
B	32178.5	32049.9	1.7947	1.7270	0.3198	0.2775
A		31818.0		1.7224		0.2887

All numerical values are in units of reciprocal centimeters.

rotational constants is inherent in the analysis of this type of MRS, since the more perturbed excited levels will often give rise to a more intense magnetic rotation feature.

The breakdown of the symmetric rotor energy formula for large values of K is illustrated in Figure 13. The addition of another term in K^4, $K^2J(J+1)$, or $J^2(J+1)^2$ to the energy formula could not improve significantly the fit to the observed transitions. As described above, the deviation from the simple formula has several possible origins and our data at present cannot distinguish among them.

Although a vibrational assignment of the entire system would be quite premature, we can tentatively assign the E, F, and G bands to have v_2 equal to 19, 20, and 21, respectively, based upon the number of sub-bands present in each vibronic band. This assignment is, we feel, consistent with our observations of the SO_2^{16} — SO_2^{18} isotope shift.

Furthermore, although there may be two or more progressions in ν_1', the main progression seems to be a rather long one in ν_2', in contrast with the assignments of Metropolis and in agreement with observations of what appears to be the analogous system in the iso-electronic SiF_2. Metropolis concluded that the intense features designated A, B, C ... by Clements were due to accidental overlapping of weak transitions rather than to a single intense progression.

Our observations with regard to the rotational fine structure and with regard to the isotope shift lead us to believe that this kind of accidental overlapping of bands contributes relatively little to the prominence of this part of the system. Preliminary Franck-Condon calculations support this position, although the excited state potential

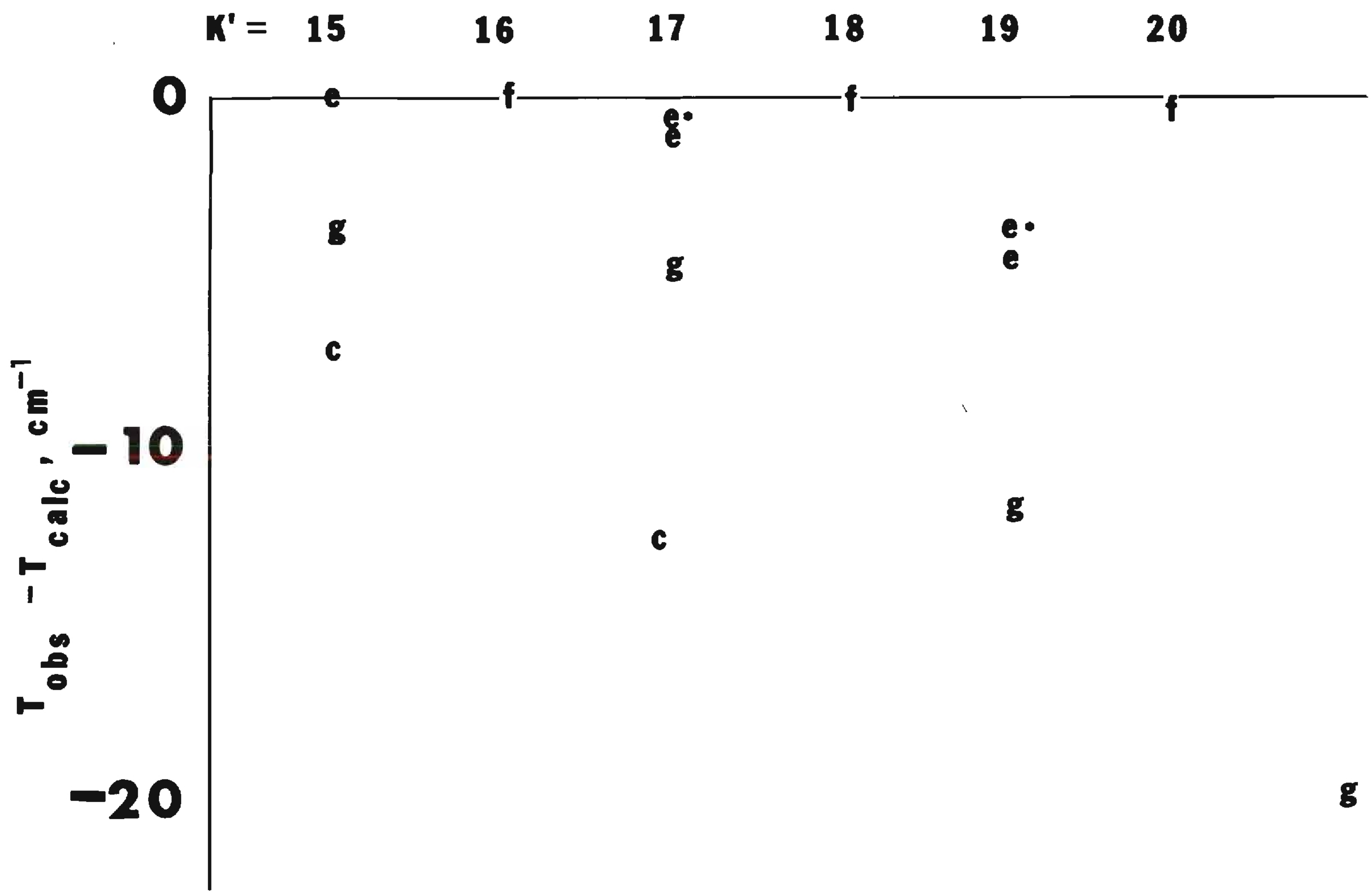
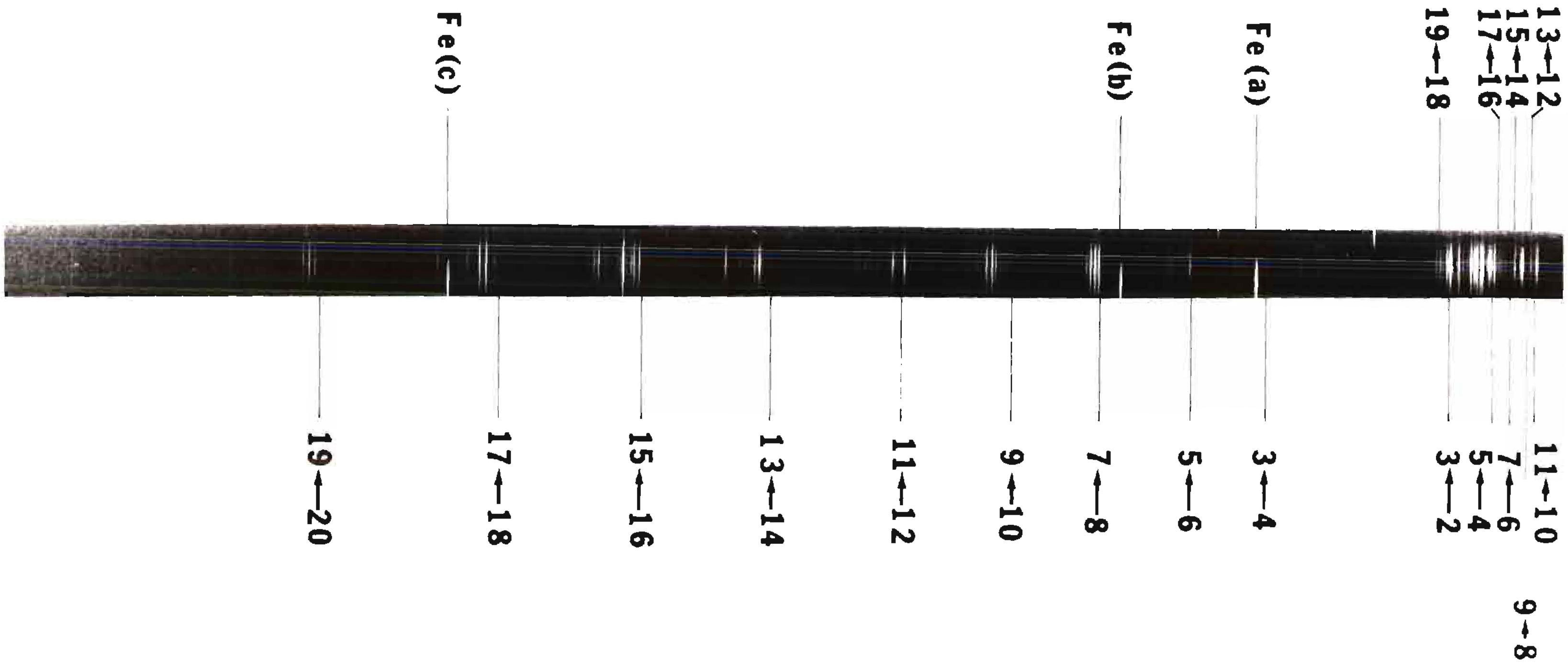


Fig. 13. Failure of the Symmetric Rotor Term Value Formulas for Several Bands of Normal and O^{18}-Enriched (*) Sulfur Dioxide.



Fe:(a) 3058.3347 Å
(b) 3059.9752
(c) 3068.1351

Fig. 14. Assignments of Leading Lines of ^{p}P and ^{r}R Branches of the SO_2^{18} E Band Demonstrating an Upper Limit to K'.

function and vibrational assignments must be understood in much greater detail before we can make a definitive statement in this respect.

Franck-Condon factors were calculated for SO_2 according to the method discussed in Appendix II. The variation of these factors with v_2 is illustrated in Figure 15. The calculated Franck-Condon factors attain a maximum at $v_2 \approx 40$; this is probably evidence for a nonlinear equilibrium geometry for the excited state, since the observed Franck-Condon maximum is at $v_2 \approx 20$ and since this maximum is much more sensitive to changes in equilibrium configuration than to changes in the curvature of the potential function.

Intensity calculations were made for the magnetic rotation spectrum assuming vanishing Zeeman splitting (considering only the magnetic rotation and circular dichroism due to field-induced mixing of the ground and excited states). The results were qualitatively quite different from our observations: progressions in J for a given K were <u>longer</u> in the calculated MRS than in absorption, and higher K' sub-bands were relatively <u>weaker</u> in the calculated MRS than in absorption. Both of these features are exactly the opposite of what is observed experimentally, as may be seen by comparing Figures 6 and 7. A typical calculated magnetic rotation spectrum is reproduced in Figure 16.

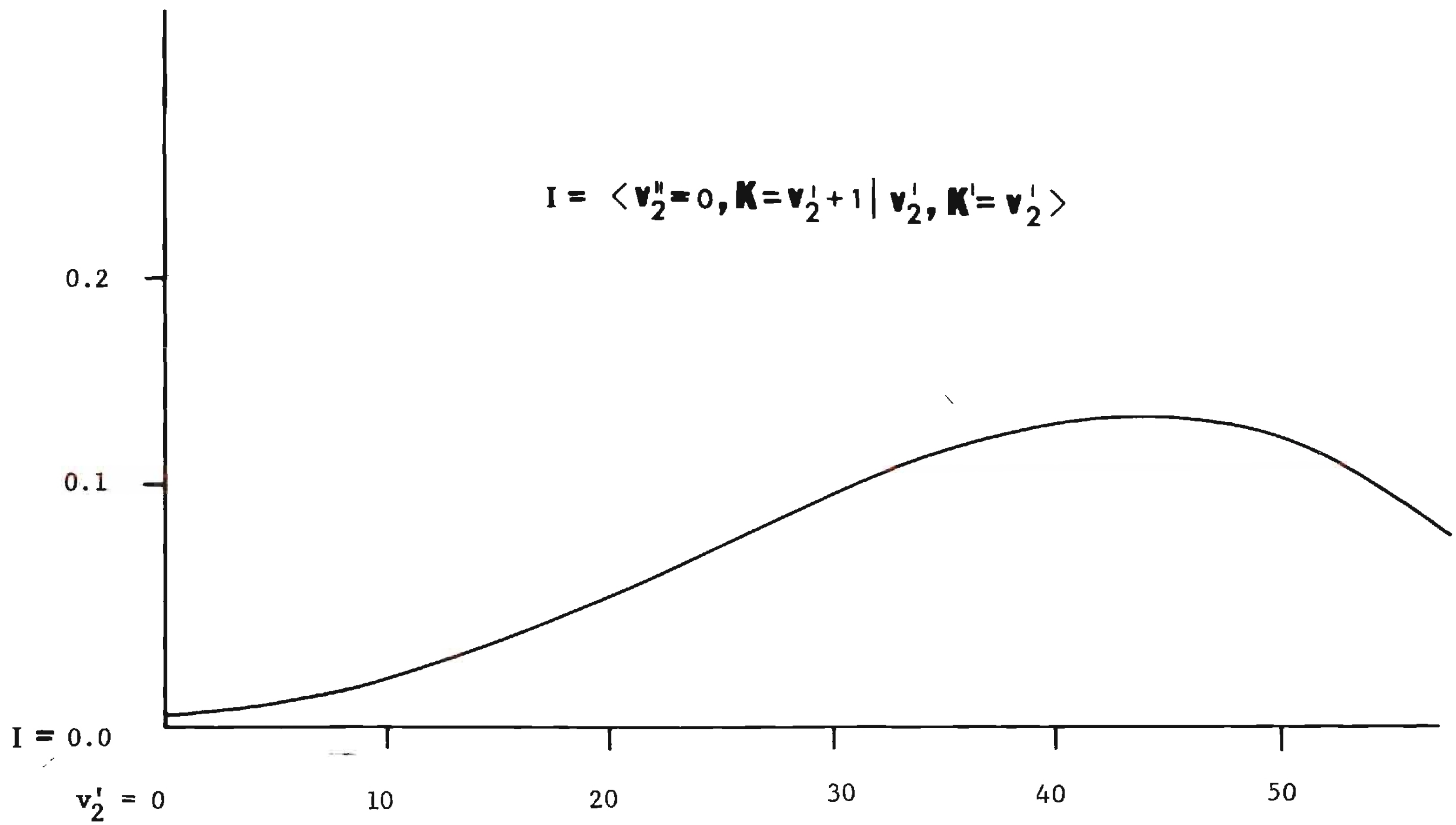


Fig. 15. Calculated Franck-Condon Factors for the $\tilde{A}\,^1B_1 \leftarrow \tilde{X}\,^1A_1$ Transition.

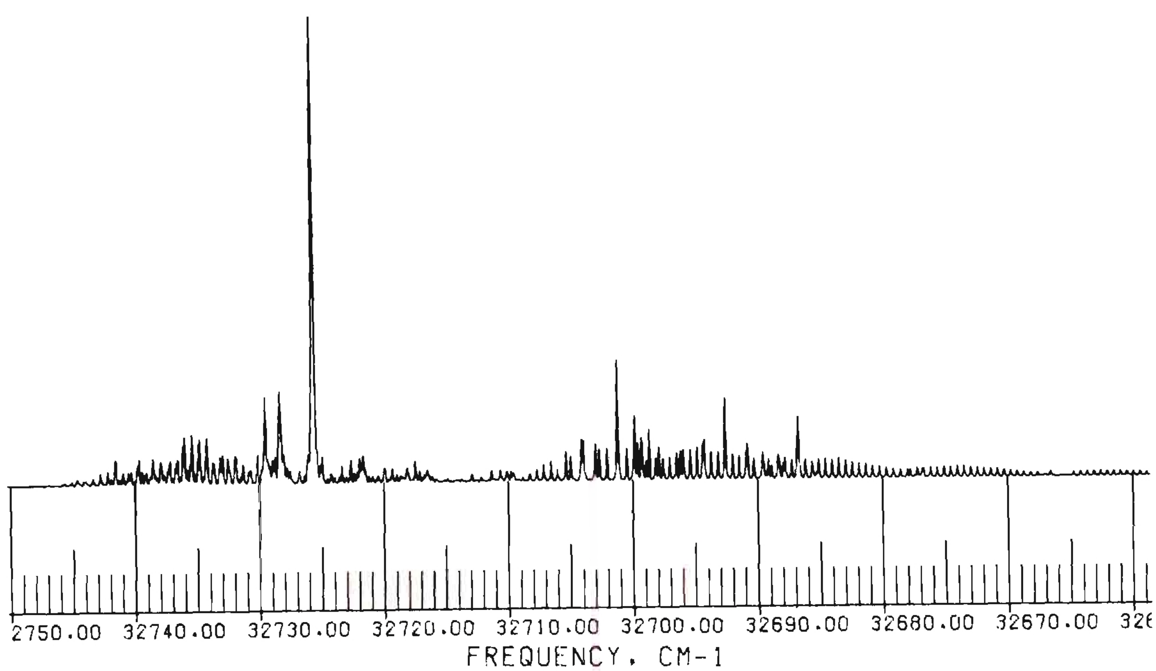


Fig. 16. Calculated Magnetic Rotation Spectrum Assuming Only Field-Induced Mixing.

CHAPTER VI

STRUCTURE OF THE EXCITED STATE

Since the bands dealt with in this analysis lie far from the system origin, the rotational constants are related only indirectly to the equilibrium geometry of the molecule. Our estimates of the equilibrium S-O bond length and angle must, therefore, be largely speculative.

The observed isotopic variation of B_v' is in reasonable accord with the assumption that the excited state is symmetric, and the two S-O bond lengths will, therefore, be treated as equal.

The values of $\left\{1/\langle\frac{1}{r^2}\rangle\right\}^{\frac{1}{2}}$ are listed in Table 2 for the E, F, G and B bands of both isotopic species. These may be corrected in a rather crude approximation by computing the expectation value for the square of the bending co-ordinate using harmonic oscillator wave-functions with v_2=230 cm^{-1} for SO_2^{16} and v_2=220 cm^{-1} for SO_2^{18}. Assuming the bond lengths do not change during the bending vibration, the bending amplitude may be used to estimate the difference between r and r_e.

This is admittedly an inconsistent way of treating the problem, since the bending amplitude is calculated as a rectilinear co-ordinate normal to the figure axis. This inconsistency is, we feel, less important than the harmonic oscillator approximation in limiting the accuracy of the calculation.

The "corrected" values of r are also included in Table 2 for comparison, and r_0 for other analyzed states of SO_2 are listed also in

Table 2. Calculated Bond Lengths For The $^1B_1$ State.

Band	$\left(1/\langle r^{-2}\rangle\right)^{1/2}$ SO_2^{16}	SO_2^{18}	$r_{corrected}$[a] SO_2^{16}	SO_2^{18}
G	1.2803Å	1.2731Å	1.3191Å	1.3116Å
F	1.2807	1.2714	1.3176	1.3082
E	1.2781	1.2747	1.3134	1.3097
B	1.2835	1.2990	1.3135	1.3287
$\tilde{a}\ ^3B_1$[b,c] r_o = 1.4926Å				
$\tilde{X}\ ^1A_1$[b,d] r_o = 1.4321Å				

a. See Text.

b. Vibrational ground state for SO_2^{16}.

c. From reference (6).

d. From reference (12).

Table 2. From consideration of the Franck-Condon effect, r_o for the $^1B_1$ state must approximate that for the $^1A_1$ ground state, or there would be long overlapping progressions in ν_1', contrary to our observations.

Although it is impossible at this point to estimate the barrier to linearity or the equilibrium bond angle, the increasing complexity of the structure of vibronic bands of energy lower than those we have analyzed suggests that it is most probable that a barrier to linearity does exist.

Molecular orbital theory, moreover, predicts unambiguously that the $^3\Sigma_g^-$ state in the linear conformation of SO_2 will be of lower energy than the $^1\Delta_g$ state. The origin of the $^3B_1$ system is 25 766 cm^{-1} (6); the linear conformation of this state is probably greater than 29 000 cm^{-1}, and the energy of the linear conformation of the $^1\Delta_g$ state must be greater than this. Since the $\tilde{A}\,^1B_1 \leftarrow \tilde{X}\,^1A_1$ system is known to extend to the red as far as 29 500 cm^{-1} (8), it is probable that these low-lying transitions are to a slightly bent state.

CHAPTER VII

DISCUSSION

This work, together with the identification of the 2300Å system of SO_2 by Srikameswaran and Brand (12) as $\tilde{C}\,^1B_2 \leftarrow \tilde{X}\,^1A_1$, can leave little doubt that the 3400-2600Å system of sulfur dioxide is the expected $\tilde{A}\,^1B_1 \leftarrow \tilde{X}\,^1A_1$ system, despite recent interpretation to the contrary (27,41). The system has many features in common with the corresponding transitions of isovalent molecules SiF_2, CF_2, CH_2, SiH_2, and HCCl (39,42,43): band systems corresponding to transitions between the two components of the $^1\Delta$ state consist mainly of long progressions in the bending frequency, and the upper component invariably has a larger bond angle. An apparent exception to the latter rule is the isoelectronic thiazyl fluoride, NSF; this anomaly has been noted by Barrow and Dixon (44), and appears to have no simple explanation.

The assignment of this system as $^1B_1$ is in good agreement with the energy of the $^1B_1$ state calculated by Hillier and Saunders (27) using Slater orbitals expanded in Gaussian functions. Those authors, however, assigned the transition incorrectly due to inadequate information concerning the rotational structure. In view of their inability to calculate accurately the transition energy to the $^3B_1$ state, this agreement is probably somewhat fortuitous.

Strictly speaking, the isotopic data and intensity arguments presented in chapter III do not rule out mixing with a triplet state, but they do increase markedly the number of unfounded assumptions one must make in order to justify such a model. The triplet state must be assumed to mix strongly with the $^1B_1$ electronic state; it must lie low enough in energy so that the interaction is uniform but high enough so that the energy denominator is unimportant; and its equilibrium geometry and potential function (of all three normal modes) must approximate that of the excited state closely enough so that the Franck-Condon factors do not get out of phase over a frequency range of 2000 cm^{-1}.

The arguments advanced in Chapter V regarding the vibrational assignment of these bands are in reasonable agreement with the recent vibrational analysis of this system by Brand and Nanes (46). These authors considered the vibrational structure of bands to the red of the A, B, C,... progression.

There are many ambiguities and contradictions which surround this analysis, and these will only be clarified by a more complete analysis of the absorption and magnetic rotation spectra and by a more rigorous molecular model. The chief problem with the present model is that it fails to predict certain similarities of magnetic field effects between the two isotopic species we have studied. Granted that the magnetic rotation spectrum is due to mixing with a quasi-continuum of ground state vibronic levels, why should this mixing be more important for the G and E bands than for the F band? If the effect were accidental in one isotopic species, it should not be observed for the other species, contrary to our observations.

A similar problem concerns the complexity of the D band. The excessive complexity of sub-band structure might indicate that more than one excited state vibrational level might be involved. The fact that it is equally complex in SO_2^{16} and SO_2^{18}, however, prevents our making such a simple explanation.

A number of known molecules are isovalent to sulfur dioxide and have the ^1A state split by an amount comparable to that in SO_2. Some of these should be expected to exhibit a magnetic rotation spectrum similar in origin to that of SO_2. They are listed in Table 3.

Table 3. Molecules Isovalent to SO_2.

Molecule	r_o''		r_o'	α_o''	α_o'	Transition Wavelength	Reference
CH_2	1.11Å		1.05Å	102.4°	≈140°	9000-4900Å	(42)
SiH_2	1.52		1.48	92.1	122	6500-4800	(43)
SiF_2	1.59		1.60	101	116	2750-2180	(42)
CF_2	1.30		1.32	104.9	122.3	2690-2400	(42)
HCF	1.12[a]	(CH)	1.12	102	127	6000-4500	(44)
	1.31	(CF)	1.30				
HCCl	1.12	(CH)	b	103	135	8200-5500	(39)
	1.69	(Cl)	b				
NSF	1.65	(SF)	1.65[a,b]	117	101[b]	4050-2150	(44)
	1.45	(SN)	1.54[b]				
HNO	1.06	(NH)	1.04	108.6	116	7700-5500	(47)
	1.21	(NO)	1.24				

[a]Assumed value.

[b]A complete rotational analysis has not been published; values are uncertain.

APPENDIX I

COMPUTER PROGRAMS

Two principal classes of computer program are described in this section: programs to handle the display of digitized spectroscopic data, and programs to relate the spectroscopic data to a specified molecular model.

Programs and Routines Available Through RECC

Several routines peculiar to the Univac 1108 or the Rich Electronic Computer Center were used in writing these programs. The most important are the Calcomp plotter routines, the NTRAN read routines, and a subroutine DGJR for inverting a real matrix in double precision.

The programs SYMBOL, AXIS, PLOT, PLOTS, and PLOTMX are copyright by Calcomp, Inc. Their description follows that given in the Georgia Institute of Technology CALCOMP User's Manual (51).

PLOTS (IBUF, IDIM, u) is a master subroutine through which all plotting subroutines are called. It must be called once and only once during the execution of any program in which plotter output is desired. IBUF is a dummy array which is used for storage of plotter input and output. "u" is an integer specifying the I/0 unit to which plotter output will be transmitted. IDIM is an integer specifying the dimension of IBUF.

PLOTMX (R) is a subroutine which terminates execution of the program if plotter output exceeds R feet in length. R is a real number.

SYMBOL (X, Y, H, RECORD, ANG, L) is a subroutine for printing alphanumeric information on a plot. The L letters or numbers contained in the variable (array) RECORD are printed on the plot beginning at co-ordinates (X, Y), printing them at a height of H inches along a line at an angle ANG from the x-direction.

PLOT (X, Y, N) causes the plotter pen to move to co-ordinate (X, Y) on the plot; if N=2, the pen is down (touching the paper); if N=3, the pen is up; if N=-3, the pen is up and the plotter co-ordinate system is transformed so that the new pen position becomes the origin of the new co-ordinate system.

AXIS (X, Y, <string>, N, XLEN, ANG, VAL, DVAL) is a subroutine which plots an axis at an angle ANG to the x-direction starting at the co-ordinate (X, Y) and continuing XLEN inches. The Hollerith alphanumeric string, <string> is printed clockwise or counterclockwise to the axis, depending on whether N is positive or negative. The absolute value of N must equal the number of characters in the Hollerith string. The subroutine also prints tic marks and a numerical scale along the axis, one number per inch. The scale starts with the value VAL and increases by an increment DVAL each inch.

NTRAN (u, ...) is a subroutine used by the UNIVAC 1108 to handle tape and disc files. NTRAN has a variable number of arguments, the first of which, u, specifies the I/O unit on which the operation is to be performed.

CALL NTRAN (u, 2, N, IDATA, ISTAT) causes a block of at most N words to be read from unit u and stored in an array IDATA of dimension N. ISTAT is a variable which has its value set equal to the number of words read if NTRAN exits normally; if NTRAN exits abnormally (due to a parity error or an end of file, for example) ISTAT is negative.

CALL NTRAN (u, 7, N) causes the unit u to skip N blocks.

CALL NTRAN (u, 22) causes the program to postpone any further execution until all NTRAN operations on unit u have been completed.

The Univac library subroutine DGJR (A, NC, NR, N, MC, $k, JC, V) is a Gauss-Jordan routine for solving a set of simultaneous linear equations (52).

A is the matrix of coefficients of the linear equations of dimension NC by NR. N is the actual number of rows used in A and MC the number of columns. The N+1th column of A contains the constant vector of the equations to be solved on input and, on output, contains the solution vector.

"k" is a statement number in the main program to which control is returned in the event of an error exit.

JC is a one-dimensional dummy array. On output, JC(1)=N if control is returned without error.

V is a one-dimensional dummy array. When V(1)=4.0 on input, simultaneous equations are solved but neither the determinent nor the inverse matrix is computed.

Data Handling Programs

The physical facilities of our laboratory and computer center are described in Chapter II. Using these facilities, we were able to store our data in digital form on magnetic tape. The information was recorded in units of 513 words per block, the first word giving the block number.

The program SCAN was written to plot the information on a digital tape on a scale that is linear in tape position (and, therefore, linear in position on the photographic plate). The digital tape is read in through I/O unit 23, and plotter output is written on unit 22.

One line of alphanumeric problem identification data is read in by the program and written as a heading on the plotter output. This feature is common to all the following programs which generate plotter output. Input parameters include the position on the photographic plate at which the scan was begun (START); the speed at which the photographic plate was scanned (SPEED); an integer, NAV, which determines the resolution with which the data is to be plotted (the subroutine AVG averages over 2^{NAV} points, as described below); and an integer ISKIP which causes the first ISKIP blocks of the digital tape not to be read. Exit from the program is accomplished by entering an end-of-file.

Characteristic output of this program follows the program listings, in Appendix IV.

```
      DIMENSION IDATA(600),IBUF(3000),IY(3500),XPOS(3500)
      DIMENSION RECORD(12)
      CALL PLOTS(IBUF,3000,22)
      CALL CHARGE
      CALL PLOTMX(120.)
      CALL PLOT(0.0,-2.0,-3)
  100 JTOT=0
      WRITE(6,171)
  171 FORMAT(' ENTER PROBLEM IDENTIFICATION DATA')
      READ(5,9,END=400)(RECORD(I),I=1,12)
    9 FORMAT(12A6)
      CALL SYMBOL(0.0,0.5,.14,RECORD,90.,72)
      CALL PLOT(1.5,0.0,-3  )
      WRITE(6,172)
  172 FORMAT(' ENTER PLATE SPEED, STARTING POSITION, NAV')
      READ(5,11,END=400)SPEED,STA ,NAV
   11 FORMAT( )
      START=STA
      CALL AXIS(0.0,2.0,18HPLATE POSITION, MM   ,-18,75.0,0.0,STA,1.0)
      DO 99 I=1,35
      DO 99 J=1,10
      P=1.0*(I-1)+0.1*J
      CALL PLOT(P,2.0,3)
      IF(J-5)96,98,96
   96 IF(J-10) 99,97,99
   97 CALL PLOT(P,2.3,2)
   98 CALL PLOT(P,2.2,2)
   99 CALL PLOT(P,2.1,2  )
      SCALE=SPEED/3600.0
      J=0
      DIDX=2.0
      PR=SCALE*(-36.5)
      YPR=4.0
  101 CALL NTRAN(23,2,600,IDATA,ISTAT)
  102 CALL NTRAN(23,22)
      IF(ISTAT)103,103,109
  103 II=ABS(ISTAT)
      GO TO (102,104,105,106),II
  104 GO TO 300
  105 CALL NTRAN(23,7,1)
      JTOT=JTOT+512
      POSN=SCALE*JTOT
      PR=SCALE*(JTOT-10)
      CALL SYMBOL(POSN,0.5,.14,26H PARITY ERROR ON A/D TAPE.  ,90.,26)
      CALL NTRAN(23,22)
      GO TO 101
  106 CALL EXIT
  109 IF(ISTAT-513)110,200,110
  110 WRITE(6,13)ISTAT
   13 FORMAT(7H ISTAT= I8)
      NR=JTOT/512
      WRITE(6,14)NR
   14 FORMAT(4H NR=  I8)
      JTOT=JTOT+ISTAT-1
      GO TO 101
  200 CONTINUE
      CALL AVG(IDATA,IY,XPOS, J,NAV,JTOT,ISTAT,SCALE)
      IF(J-2990)101,101,220
C
```

```
C       PLOT THE OBSERVED SPECTRUM
C
  220 CALL PLOT(POSN,YINT,3)
      DO 221 I=1,J
      POSN=XPOS(I)
      YINT=IY(I)*.002
  221 CALL PLOT(POSN,YINT,2)
C
C       PLOT THE DERIVATIVE OF THE SPECTRUM
C
C
      CALL PLOT(PR,DIDX,3)
      DO 222 I=1,J
      POSN=XPOS(I)
      YINT=IY(I)*.002
      DIDX=(YINT-YPR)/((POSN-PR)*100.)
      D=ABS(DIDX)
      DIDX=DIDX+2.0
      YPR=YINT
      PR=POSN
      IF(D-1.5)2210,222,2220
 2220 DIDX=2.0
 2210 CALL PLOT(POSN,DIDX,2)
  222 CONTINUE
    1 J=0
      GO TO 101
  300 CALL PLOT(POSN,YINT,3)
      DO 321 I=1,J
      POSN=XPOS(I)
      YINT=IY(I)*.002
  321 CALL PLOT(POSN,YINT,2)
      CALL PLOT(PR,DIDX,3)
      DO 322 I=1,J
      POSN=XPOS(I)
      YINT=IY(I)*.002
      DIDX=(YINT-YPR)/((POSN-PR)*100.)
      D=ABS(DIDX)
      DIDX=DIDX+2.0
      YPR=YINT
      PR=POSN
      IF(D-1.5)3210,322,3221
 3221 DIDX=2.0
 3210 CALL PLOT(POSN,DIDX,2)
  322 CONTINUE
 3220 CALL PLOT(POSN,YINT, 999        )
      GO TO 100
  400 CALL EXIT
      END
```

SCAN calls the subroutines AVG (version 1), and CHARGE. CHARGE is a subroutine which causes plotter output to be charged to the appropriate account number. It is not listed here.

AVG (IDATA, IY, XPOS, J, NAV, JTOT, ISTAT, SCALE) determines the resolution with which the spectrum will be plotted. This subroutine averages 2^{NAV} consecutive points and plots them as a single point at their average position along the x and y axes (XPOS and YPOS). This subroutine derives its usefulness from the fact that the digital sampling rate ordinarily exceeds the limits of resolution determined by the grain size of the photographic plate.

```
      SUBROUTINE AVG(IDATA,IY,XPOS,J,NAV,JTOT,ISTAT,SCALE)
      DIMENSION IY(3500),XPOS(3500),IDATA(600)
      NMAX=2**NAV
      NSI=1
  100 J=J+1
      SUMY=0.0
      DO 101 I=1,NMAX
      K=NSI+I
  101 SUMY=SUMY+(1.0*IDATA(K))
      SUMY=SUMY/(1.0*NMAX)
      IY(J)=SUMY
      XPOS(J)=JTOT*SCALE+NST*SCALE+NMAX*SCALE*0.5
      XPOS(J)=ABS(XPOS(J))
      NST=NST+NMAX
      IF(ISTAT-NST)200,200,100
  200 JTOT=JTOT+ISTAT-1
      RETURN
      END
```

XPAND is a scale expansion program used for expanding segments of a plot obtained by the program SCAN. Input consists of the problem identification data, plate speed, and starting position as required for SCAN; YMIN and YMAX, the approximate values in inches of the minimum and maximum position along the y-axis plotted by SCAN (if YMIN and YMAX are interchanged, the sense of the spectrum is reversed); and the first and last point along the x-axis of each segment to be expanded. Execution is terminated by entering the pair of points (777.,777.).

XPAND calls the subroutines CHARGE and DAMP.

```
      DIMENSION RECORD(12)
      DIMENSION IDATA(600),IBUF(3000),IY(3000),XPOS(3000)
      CALL PLOTS(IBUF,3000,22)
      CALL CHARGE
      CALL PLOT(0.0,-3.0,-3)
      WRITE(6,170)
  170 FORMAT(' ENTER PROBLEM IDENTIFICATION DATA')
      READ(5,9)(RECORD(I),I=1,12)
    9 FORMAT(12A6)
      CALL SYMBOL(0.0,0.5,.14,RECORD,90.,72)
      CALL PLOT(1.5,0.0,-3)
  100 JTOT=0
      JQ=0
      WRITE(6,171)
  171 FORMAT(' ENTER PLATE SPEED, STARTING POSN, YMIN, YMAX')
      READ(5,11)SPEED,STA,YMIN,YMAX
   11 FORMAT()
      START=STA
      IF(YMIN)90,90,91
   90 YMIN=4.0
      YMAX=8.0
   91 YRANGE=YMAX-YMIN
      SCALE=SPEED/3600.0
      WRITE(6,172)
  172 FORMAT(' ENTER FIRST AND LAST POINT OF SEGMENT TO BE EXPANDED'
     2/' EXIT WITH 777.')
   94 READ(5,11)P1,P2
      IF(P1-777.0)95,909,95
   95 DP=ABS(P1-P2)
      DP=10.*DP
      DP=DP+1
      IDP=DP
      PI=P1*10.
      IP=PI
      PI=IP/10.
      PJ=P2*10.
      JP=PJ
      PJ=JP/10.
      P0=P1-START
      P0=P0/(SCALE*512)
      ISKIP=P0
      ISKIP=ISKIP-JQ
      CALL NTRAN(23,7,ISKIP)
      JTOT=JTOT+ISKIP*512
      JQ=JQ+ISKIP
      CALL AXIS(0.0,4.0,18HPLATE POSITION, MM  ,-18,DP,0.0,PI,0.1)
      DO 99 I=1,IDP
      DO 99 J=1,10
      P=1.0*(I-1)+0.1*J
      CALL PLOT(P,4.0,3)
      IF(J-5)96,98,96
   96 IF(J-10) 99,97,99
   97 CALL PLOT(P,5.0,2)
   98 CALL PLOT(P,4.5,2)
   99 CALL PLOT(P,4.3,2)
      J=0
      DIDX=2.0
      PR=SCALE*(-36.5)
      YPR=4.5
```

```
      CALL NTRAN(23,22)
  101 CALL NTRAN(23,2,600,IDATA,ISTAT)
      JQ=JQ+1
  102 CALL NTRAN(23,22)
      IF(ISTAT)103,103,200
  103 II=ABS(ISTAT)
      GO TO (102,104,105,106),II
  104 GO TO 300
  105 CALL NTRAN(23,7,1)
      JTOT=JTOT+512
      POSN=SCALE*JTOT
      CALL NTRAN(23,22)
      GO TO 101
  106 CALL EXIT
  200 SUMY=0.0
      J=J+1
      DO 211 I=2,74
  211 SUMY=1.0*IDATA(I)+SUMY
      IY(J)=SUMY/73.0
      XPOS(J)=JTOT*SCALE+SCALE*36.5
      J=J+1
      SUMY=0.0
      IF(XPOS(J)+START-PJ)2011,300,300
 2011 CONTINUE
      DO 212 I=75,147
  212 SUMY=1.0*IDATA(I)+SUMY
      IY(J)=SUMY/73.0
      XPOS(J)=JTOT*SCALE+SCALE*109.5
      J=J+1
      SUMY=0.0
      IF(XPOS(J)+START-PJ)2012,300,300
 2012 CONTINUE
      DO 213 I=148,220
  213 SUMY=1.0*IDATA(I)+SUMY
      IY(J)=SUMY/73.0
      XPOS(J)=JTOT*SCALE+SCALE*182.5
      J=J+1
      SUMY=0.0
      IF(XPOS(J)+START-PJ)2013,300,300
 2013 CONTINUE
      DO 214 I=221,293
  214 SUMY=1.0*IDATA(I)+SUMY
      IY(J)=SUMY/73.0
      XPOS(J)=JTOT*SCALE+SCALE*255.5
      J=J+1
      SUMY=0.
      IF(XPOS(J)+START-PJ)2014,300,300
 2014 CONTINUE
      DO 215 I=294,366
  215 SUMY=1.0*IDATA(I)+SUMY
      IY(J)=SUMY/73.0
      XPOS(J)=JTOT*SCALE+SCALE*328.5
      J=J+1
      SUMY=0.
      IF(XPOS(J)+START-PJ)2015,300,300
 2015 CONTINUE
      DO 216 I=367,439
  216 SUMY=1.0*IDATA(I)+SUMY
      IY(J)=SUMY/73.0
      XPOS(J)=JTOT*SCALE+SCALE*401.5
```

```
      J=J+1
      SUMY=0.
      DO 217 I=440,512
      IF(XPOS(J)+START-PJ)2016,300,300
 2016 CONTINUE
  217 SUMY=1.0*IDATA(I)+SUMY
      IY(J)=SUMY/73.0
      XPOS(J)=JTOT*SCALE+SCALE*474.5
      JTOT=JTOT+ISTAT-1
      IF(XPOS(J)+START-PJ)2017,300,300
 2017 CONTINUE
      IF(J-2990)101,101,220
C
C       PLOT THE OBSERVED SPECTRUM
C
  220 CALL PLOT(POSN,2.0 ,3)
      CALL DAMP(IY,J)
      DO 221 I=1,J
      POSN=(XPOS(I)+START-PI)*10.0
      YINT=IY(I)*.002
      YINT=4.0+(YINT-YMIN)*4.0/YRANGE
  221 CALL PLOT(POSN,YINT,2)
C
C       PLOT THE DERIVATIVE OF THE SPECTRUM
C
      PR=  (XPOS(1)+START-PI)*10.0
      YPR=IY(1)*.004
      CALL PLOT(PR,4.0 ,3)
      J=J-1
      DO 222 I=2,J
      POSN=(XPOS(I)+START-PI)*10.0
      YINT=IY(I+1)*.004
      DIDX=(YINT-YPR)/((POSN-PR)*15.0)
      DIDX=DIDX*(4.0/YRANGE)
      D=ABS(DIDX)
      DIDX=DIDX+4.0
      YPR =IY(I)*.004
      PR=POSN
      IF(D-3.0)2210,222,222
 2210 CALL PLOT(POSN,DIDX,2)
  222 CONTINUE
      J=0
      GO TO 101
  300 CALL PLOT(POSN,2.0 ,3)
      CALL DAMP(IY,J)
      DO 321 I=1,J
      POSN=(XPOS(I)+START-PI)*10.0
      YINT=IY(I)*.002
      YINT=4.0+(YINT-YMIN)*4.0/YRANGE
  321 CALL PLOT(POSN,YINT,2)
      CALL PLOT(PR,4.0 ,3)
      PR=  (XPOS(1)+START-PI)*10.0
      YPR=IY(1)*.004
      J=J-1
      DO 322 I=2,J
      POSN=(XPOS(I)+START-PI)*10.0
      YINT=IY(I+1)*.004
      DIDX=(YINT-YPR)/((POSN-PR)*15.0)
      DIDX=DIDX*(4.0/YRANGE)
      D=ABS(DIDX)
```

```
      DIDX=DIDX+4.0
      YPR =IY(I)*.004
      PR=POSN
      IF(D-3.0)3210,322,322
 3210 CALL PLOT(POSN,DIDX,2)
  322 CONTINUE
      CALL PLOT(POSN+3.5,0.0,-3)
      POSN=0.0
      GO TO 94
  909 CALL PLOT(POSN,YINT, 999        )
      END
```

DAMP is a subroutine which damps signal oscillations by computing a point-simultaneous weighted average of neighboring data points. Output is stored in the same array as input.

```
      SUBROUTINE DAMP(N,J)
      DIMENSION N(3000),B(3000)
C
C     THIS SUBROUTINE DAMPS SIGNAL OSCILLATIONS USING A WEIGHTED
C     RUNNING AVERAGE
C
      J=J-1
      DO 200 I=2,J
  200 B(I)=.5*N(I)+.25*(N(I-1)+N(I+1))
      DO 300 I=2,J
  300 N(I)=B(I)
      J=J+1
      RETURN
      END
```

The programs SPLOT and MPLOT both plot the observed spectrum on a scale that is linear in frequency; for SPLOT the scale is 1 cm^{-1} per inch, and for MPLOT the scale is 10 cm^{-1} per inch. Since the two programs are quite similar, a listing of SPLOT is presented in a form that is convenient for batch processing, while MPLOT is presented in an interactive form convenient for demand (time sharing) processing.

Both programs call the subroutines CHARGE and DAMP (described above). In addition, they use the subroutines AVG (version 2), TIC, and SIGN.

Input for the program consists of the problem identification data, starting point, plate speed, ISKIP, and NAV (as given in XPAND), and the coefficients of the cubic equation relating plate position to vacuum wavelength (as obtained from SCALE).

```
      COMMON JOKER,STARTI
      DOUBLE PRECISION P1,P2
      DIMENSION RECORD(12),IDATA(600),XPOS(3000),IY(3000),IBUF(3000)
      CALL NTRAP
      CALL PLOTS(IBUF,3000,22)
      CALL PLOT(0.0,-3.0,-3)
  100 READ(5,10)(RECORD(I),I=1,12)
   10 FORMAT(12A6)
      CALL SYMBOL(0.0,0.5,.14,RECORD,90.,72)
      CALL PLOT(1.5,0.2,-3)
      READ(5,11)START,SPEED,NAV,ISKIP,YMIN,YMAX
   11 FORMAT(2F12.6,2I8,2F12.6)
      IF(YMIN)98,98,99
   98 YMIN=4.0
      YMAX=8.0
   99 YRANGE=YMAX-YMIN
      CALL NTRAN(23,7,ISKIP)
      JTOT=512*ISKIP
      READ(5,12)ACON,BCON,CCON,DCON
   12 FORMAT(4F15.6)
      SCALE=SPEED/3600.0
      P1=START
      P1=ACON*(P1**3)+BCON*(P1**2)+CCON*P1+DCON
      P1=(10.0**8)/P1
      KK=P1
      STARTI=KK
      CALL TIME(B,I1)
      P2=START+(36.5*SCALE)
      P2=ACON*(P2**3)+BCON*(P2**2)+CCON*P2+DCON
      P2=(10.0**8)/P2
      CALL TIME(B,I2)
      IT=I2-I1
      WRITE(6,13)P1,P2
   13 FORMAT(4H P1= F12.6/4H P2= F12.6)
      WRITE(6,14)IT
   14 FORMAT(6H TIME=  I5)
      CALL SIGN(P1,P2,JOKER)
      XI=0.0
      J=0
  101 CALL NTRAN(23,2,600,IDATA,ISTAT)
  102 CALL NTRAN(23,22)
      IF(ISTAT)103,103,200
  103 II=ABS(ISTAT)
      GO TO (102,104,105,106),II
  104 GO TO 300
  105 CALL NTRAN(23,7,1)
      JTOT=JTOT+512
      POSN=SCALE*JTOT
      P=POSN
      POSN=ACON*(P**3)+BCON*(P*P)+CCON*P+DCON
      POSN=10.0**8/POSN
      CALL NTRAN(23,22)
      GO TO 101
  106 CALL EXIT
  200 IF(ISTAT-513)201,202,201
  201 WRITE(6,22)ISTAT
   22 FORMAT(I8)
  202 CALL AVG(IY,XPOS,JTOT,SCALE,NAV,J,IDATA,ISTAT,ACON,BCON,CCON,DCON,
     1START)
      IF(J-1000)101,101,220
  220 POSN=XHOLD
      YINT=YHOLD
```

```
      CALL PLOT(POSN,YINT,3)
      CALL DAMP(IY,J)
C
C     PLOT THE OBSERVED SPECTRUM
C
      DO 221 I=1,J
      POSN=XPOS(I)
      YINT=IY(I)*.002
      YINT=4.0+(YINT-YMIN)*4.0/YRANGE
  221 CALL PLOT(POSN,YINT,2)
      XHOLD=POSN
      YHOLD=YINT
      CALL PLOT(PR,DIDX,3)
C
C     PLOT THE DERIVATIVE OF THE SPECTRUM
C
      CALL DAMP(IY,J)
      J=J-1
      DO 222 I=2,J
      POSN=XPOS(I)
      YINT=IY(I+1)*.004
      DIDX=(YINT-YPR)/((POSN-PR)*40.0)
      DIDX=DIDX*(4.0/YRANGE)
      D=ABS(DIDX)
      DIDX=DIDX+3.0
      YPR=IY(I)*.004
      PR=POSN
      IF(D-3.0)2210,222,222
 2210 CALL PLOT(POSN,DIDX,2)
  222 CONTINUE
      J=J+1
C
C     PLOT THE X AXIS
C
      KK=XPOS(J)
      XF=KK
      XLEN=XF-XI
      XVAL=STARTI+XI*JOKER
      DEC=JOKER
      CALL AXIS(XI,3.0,15HFREQUENCY, CM-1,-15,XLEN,0.0,XVAL,DEC)
      CALL TIC(XI,XF)
      XI=XF
      J=0
      GO TO 101
  300 CONTINUE
      POSN=XHOLD
      YINT=YHOLD
      CALL DAMP(IY,J)
  320 CALL PLOT(POSN,YINT,3)
      DO 321 I=1,J
      POSN=XPOS(I)
      YINT=4.0+(YINT-YMIN)*4.0/YRANGE
      YINT=IY(I)*.002
  321 CALL PLOT(POSN,YINT,2)
      CALL PLOT(PR,DIDX,3)
      CALL DAMP(IY,J)
      J=J-1
```

```
      DO 322 I=2,J
      POSN=XPOS(I)
      YINT=IY(I+1)*.004
      DIDX=(YINT-YPR)/((POSN-PR)*40.0)
      DIDX=DIDX*(4.0/YRANGE)
      D=ABS(DIDX)
      DIDX=DIDX+3.0
      YPR=IY(I)*.004
      PR=POSN
      IF(D-3.0)3210,322,322
 3210 CALL PLOT(POSN,DIDX,2)
  322 CONTINUE
      J=J+1
C
C     PLOT THE X AXIS
C
      KK=XPOS(J)
      XF=KK+1
      XLEN=XF-XI
      XVAL=STARTI+XI*JOKER
      DEC=JOKER
      CALL AXIS(XI,3.0,15HFREQUENCY, CM-1,-15,XLEN,0.0,XVAL,DEC)
      CALL TIC(XI,XF)
      CALL PLOT(XF,0.0,999)
      CALL EXIT
      END
```

```
      COMMON JOKER,STARTI
      DOUBLE PRECISION P1,P2
      DIMENSION RECORD(12),IDATA(600),XPOS(3000),IY(3000),IBUF(3000)
      CALL PLOTS(IBUF,3000,22)
      CALL CHARGE
      CALL PLOTMX(300.)
      CALL PLOT(0.0,-3.0,-3)
      JTOT=0
      WRITE(6,171)
  171 FORMAT(' ENTER PROBLEM IDENTIFICATION DATA.')
  100 READ(5,10)(RECORD(I),I=1,12)
   10 FORMAT(12A6)
      CALL SYMBOL(0.0,0.5,.14,RECORD,90.,72)
      CALL PLOT(1.5,0.2,-3)
      WRITE(6,172)
  172 FORMAT(' ENTER START, SPEED, NAV, ISKIP, YMIN, YMAX')
      READ(5,11)START,SPEED,NAV,ISKIP,YMIN,YMAX
   11 FORMAT()
      IF(YMIN)98,98,99
   98 YMIN=4.0
      YMAX=8.0
   99 YRANGE=YMAX-YMIN
      CALL NTRAN(23,7,ISKIP)
      JTOT=512*ISKIP
      WRITE(6,173)
  173 FORMAT(' ENTER CUBIC, QUADRATIC, LINEAR, CONSTANT COEFFICIENTS')
      READ(5,12)ACON,BCON,CCON,DCON
   12 FORMAT()
      SCALE=SPEED/3600.0
      P1=START+SCALE*JTOT
      P1=ACON*(P1**3)+BCON*(P1**2)+CCON*P1+DCON
      P1=(10.0**8)/P1
      KK=P1
      STARTI=KK
      P2=START+((JTOT+(2**NAV))*SCALE)
      P2=ACON*(P2**3)+BCON*(P2**2)+CCON*P2+DCON
      P2=(10.0**8)/P2
      WRITE(6,13)P1,P2
   13 FORMAT(4H P1= F12.6/4H P2= F12.6)
      CALL SIGN(P1,P2,JOKER)
      XI=0.0
      J=0
  101 CALL NTRAN(23,2,600,IDATA,ISTAT)
  102 CALL NTRAN(23,22)
      IF(ISTAT)103,103,200
  103 II=ABS(ISTAT)
      GO TO (102,104,105,106),II
  104 GO TO 300
  105 CALL NTRAN(23,7,1)
      WRITE(6,14)POSN
   14 FORMAT(' PARITY AT',F12.3)
      JTOT=JTOT+512
      POSN=SCALE*JTOT
      P=POSN
      POSN=ACON*(P**3)+BCON*(P*P)+CCON*P+DCON
      POSN=10.0**8/POSN
      CALL NTRAN(23,22)
      GO TO 101
  106 CALL EXIT
```

```
  200 IF(ISTAT-513)201,202,201
  201 WRITE(6,22)ISTAT
   22 FORMAT(I8)
  202 CALL AVG(IY,XPOS,JTOT,SCALE,NAV,J,IDATA,ISTAT,ACON,BCON,CCON,DCON,
     1START)
      IF(J-1000)101,101,220
  220 POSN=XHOLD
      YINT=YHOLD
      CALL PLOT(POSN,YINT,3)
      CALL DAMP(IY,J)
C
C     PLOT THE OBSERVED SPECTRUM
C
      DO 221 I=1,J
      POSN=XPOS(I)
      YINT=IY(I)*.002
      YINT=4.0+(YINT-YMIN)*4.0/YRANGE
  221 CALL PLOT(POSN,YINT,2)
      XHOLD=POSN
      YHOLD=YINT
      CALL PLOT(PR,DIDX,3)
C
C     PLOT THE DERIVATIVE OF THE SPECTRUM
C
      CALL DAMP(IY,J)
      J=J-1
      DO 222 I=2,J
      POSN=XPOS(I)
      YINT=IY(I+1)*.004
      DIDX=(YINT-YPR)/((POSN-PR)*40.0)
      DIDX=DIDX*(4.0/YRANGE)
      D=ABS(DIDX)
      DIDX=DIDX+3.0
      YPR=IY(I)*.004
      PR=POSN
      IF(D-3.0)2210,222,222
 2210 CALL PLOT(POSN,DIDX,2)
  222 CONTINUE
      J=J+1
C
C     PLOT THE X AXIS
C
      KK=XPOS(J)
      XF=KK
      XLEN=XF-XI
      XVAL=STARTI+XI*JOKER
      DEC=JOKER
      CALL AXIS(XI,3.0,15HFREQUENCY, CM-1,-15,XLEN,0.0,XVAL,DEC)
      CALL TIC(XI,XF)
      XI=XF
      J=0
      GO TO 101
  300 CONTINUE
      POSN=XHOLD
      YINT=YHOLD
      CALL DAMP(IY,J)
  320 CALL PLOT(POSN,YINT,3)
      DO 321 I=1,J
      POSN=XPOS(I)
      YINT=4.0+(YINT-YMIN)*4.0/YRANGE
```

```
      YINT=IY(I)*.002
  321 CALL PLOT(POSN,YINT,2)
      CALL PLOT(PR,DIDX,3)
      CALL DAMP(IY,J)
      J=J-1
      DO 322 I=2,J
      POSN=XPOS(I)
      YINT=IY(I+1)*.004
      DIDX=(YINT-YPR)/((POSN-PR)*40.0)
      DIDX=DIDX*(4.0/YRANGE)
      D=ABS(DIDX)
      DIDX=DIDX+3.0
      YPR=IY(I)*.004
      PR=POSN
      IF(D-3.0)3210,322,322
 3210 CALL PLOT(POSN,DIDX,2)
  322 CONTINUE
      J=J+1
C
C     PLOT THE X AXIS
C
      KK=XPOS(J)
      XF=KK+1
      XLEN=XF-XI
      XVAL=STARTI+XI*JOKER
      DEC=JOKER
      CALL AXIS(XI,3.0,15HFREQUENCY, CM-1,-15,XLEN,0.0,XVAL,DEC)
      CALL TIC(XI,XF)
      CALL PLOT(XF,0.0,999)
      CALL EXIT
      END
```

AVG (IY, XPOS, JTOT, SCALE, NAV, J, IDATA, ISTAT, ACON, BCON, CCON, DCON, START) (version 2), in addition to performing the function of AVG (version 1), computes the vacuum frequency associated with each data point.

```
      SUBROUTINE AVG(IY,XPOS,JTOT,SCALE,NAV,J,IDATA,ISTAT,A,B,C,D,ST)
      COMMON JOKER,STARTI
      DIMENSION IY(3000),XPOS(3000),IDATA(600)
      NMAX=2**NAV
      NST=1
  100 J=J+1
      SUMY=0.0
      DO 101 I=1,NMAX
      K=NST+I
  101 SUMY=SUMY+(1.0*IDATA(K))
      SUMY=SUMY/(1.0*NMAX)
      IY(J)=SUMY
      XPOS(J)=JTOT*SCALE+NST*SCALE+NMAX*SCALE*0.5+ST
      X=XPOS(J)
      X=A*X*X*X+B*X*X+C*X+D
      XPOS(J)=(10**8)/X
      XPOS(J)=(XPOS(J)-STARTI)*JOKER
      NST=NST+NMAX
      IF(ISTAT-NST)200,200,100
  200 JTOT=JTOT+ISTAT-1
      RETURN
      END
```

TIC (XI, XF) is a subroutine which causes tic marks to be drawn every .1 inches along the x-axis of the plot between XI and XF. Tic marks at half-inch and one-inch intervals are drawn longer than others.

```
      SUBROUTINE TIC(XI,XF)
C
C     THIS SUBROUTINE DRAWS TIC MARKS ON THE SCALE EVERY .1 INCHES
C
      DX=XI-XF
      DX=ABS(DX)
      IDX=DX
      DO 99 I=1,IDX
      DO 99 J=1,10
      P=1.0*(I-1)+0.1*J+XI
      CALL PLOT(P,3.0,3)
      IF(J-5)96,98,96
   96 IF(J-10) 99,97,99
   97 CALL PLOT(P,4.0,2)
   98 CALL PLOT(P,3.5,2)
   99 CALL PLOT(P,3.3,2)
      RETURN
      END
```

SIGN (P1, P2 JOKER) determines whether the energy scale is increasing (JOKER is set equal to 1) or decreasing (JOKER is set equal to -1).

```
      SUBROUTINE SIGN(P1,P2,JOKER)
C
C     THIS SUBROUTINE DETERMINES WHETHER THE ENERGY SCALE IS
C     INCREASING OR DECREASING AND RETURNS THIS INFORMATION VIA
C     THE VARIABLE JOKER
C
      P0=P2-P1
      IF(P0)101,901,102
  101 JOKER=-1
      GO TO 909
  102 JOKER=1
      GO TO 909
  901 WRITE(6,90)
   90 FORMAT(6H ERROR/6H ERROR/6H ERROR/14H SCALE IS ZERO )
      CALL PLOT(0.0,0.0,999)
      CALL EXIT
  909 RETURN
      END
```

The program SCALE uses the relative positions (measured in mm along the photographic plate as obtained from the output of XPAND) of the iron calibration lines on the digital tape and fits their vacuum wavelengths to a cubic equation in relative position. Input includes the relative position of each calibration line and its vacuum wavelength; the number of unknowns (4) and the number of iterations to achieve the desired accuracy (usually set to 1). Output consists of the calculated coefficients of the cubic equation $\lambda=Ax^3+Bx^2+Cx+D$; and the observed and calculated vacuum wavelength of each calibration line, along with their difference.

SCALE calls the library subroutine DGJR described above.

```
      IMPLICIT DOUBLE PRECISION (D)
      DIMENSION V(50),F(50,10),DF(10,10),JC(1),DV(2),
     2          FC(50),FD(50),FO(50),DX(10)
    5 WRITE (6,10)
   10 FORMAT('  ENTER POSN, WAVELENGTH, NEG.FLAG')
   15 I=0
   20 I=I+1
      READ (5,25) V(I),FO(I)
   25 FORMAT ( )
      IF (V(I).GE.0) GO TO 20
      I=I-1
   30 WRITE (6,35)
   35 FORMAT(' THANK YOU.'/' ENTER NO. UNKNOWNS, NO. ITER.')
      READ (5,40) N,IT
   40 FORMAT ( )
      IF (IT.LE.0) GO TO 999
      DO 45 J=1,I,1
      DO 45 K=1,N,1
   45 F(J,K)=V(J)**(K-1)
      DO 65 J=1,N,1
      DA=0.0D0
      DO 55 K=J,N,1
      DB=0.0D0
      DO 50 L=1,I,1
   50 DB=DB+F(L,K)*F(L,J)
      DF(J,K)=DB
   55 DF(K,J)=DB
      DO 60 K=1,I,1
   60 DA=DA+F(K,J)*FO(K)
   65 DF(J,N+1)=DA
```

```
      IC=0
   70 DV(1)=6.0
      IC=IC+1
      CALL DGJR (DF,10,10,N,N+1,$115,JC,DV)
      DO 80 J=1,I,1
      DA=0.0D0
      DO 75 K=1,N,1
   75 DA=DA+F(J,K)*DF(K,N+1)
      FC(J)=DA
   80 FD(J)=FO(J)-DA
      IF (IT-IC.LE.0) GO TO 95
      DO 90 J=1,N,1
      DA=0.0D0
      DO 85 K=1,I,1
   85 DA=DA+F(K,J)*FD(K)
      DX(J)=DF(J,N+1)
   90 DF(J,N+1)=DA
      GO TO 70
   95 DO 100 J=1,N,1
  100 DF(J,N+1)=DF(J,N+1)+DX(J)
      WRITE (6,105) ((V(J),FO(J),FC(J),FD(J)),J=1,I,1)
  105 FORMAT(' POSITION   OBS WAVELENGTH   CALC WAVELENGTH',
     2 '    DIFFERENCE',50(/F9.4,F18.6,F18.6,F12.6))
      WRITE (6,110) (DF(J,N+1),J=1,N,1)
  110 FORMAT(' D=',F17.9,/' C=',F17.12/' B=',F17.12/
     2 ' A=',F17.12)
  115 WRITE (6,120) JC,DV(1),DV(2)
  120 FORMAT (1H0,'JC =',I3,5X,'DV(1) =',D15.8,5X,
     2          'DV(2) =',D15.8)
      IF (FO(I+1).GE.0) GO TO 5
  200 WRITE(6,21)
   21 FORMAT(' ENTER POSITION')
      READ(5,25)P
      IF(P)999,201,201
  201 W=DF(1,5)+DF(2,5)*P+DF(3,5)*P*P+DF(4,5)*P*P*P
      FREQ=(10.**8)/W
      WRITE(6,22)FREQ,W
   22 FORMAT(' FREQUENCY=',F12.3,'  WAVELENGTH=',F12.4)
      GO TO 200
  999 STOP
      END
```

Model Calculations

The most important programs used in fitting the spectroscopic data to a molecular model were FIT and ODDFIT. These programs read in assigned J', K', J", and K" values for a given transition frequency, retrieve ground state rotational term values for the molecule of interest, compute excited state term values and fit these term values to a symmetric top energy formula. Since the model for the excited state is a linear molecule, each vibronic band will have only even or odd values of K' associated with it. FIT was used for vibronic bands with even K', and ODDFIT was used for bands with odd K'.

Input includes the assigned transitions, the ground state rotational term values (read in via NTRAN), and a series of control statements to determine the sequence of operations.

The operator may calculate excited state rotational constants after entering any number of assignments (up to 100) by entering an assignment with $J' < 0$. The program then will calculate coefficients of $J(J+1)$, K^2, K^4, $K^2J(J+1)$, and $J^2(J+1)^2$, at the option of the operator.

The program returns as output the calculated rotational constants, the root mean square deviation, and, for each assignment, the observed frequency, calculated frequency, and frequency difference. Assignments may then be changed by entering the number of the assignments to be changed and the revised values of J', K', J", K", and frequency. This section of the program may be exited from by entering a negative value for the assignment index.

Since the most prominent types of transitions encountered in the spectrum of SO_2 are ^pP and ^rR branches, these programs were written only to accommodate assignments corresponding to these two types of branch.

Once revised assignments are entered, the operator may choose to recalculate the rotational constants, to enter further assignments, to print the calculated positions of all lines with $0 \leq K' < 20$ and $K' \leq J' \leq K'+10$, or to dump these calculated positions into a data file. If one of the first two options is chosen, the first segment of the program is re-entered, and the program begins the input cycle with the last assignment previously entered.

```
      DOUBLE PRECISION A,ATA,ATY,X,Y,A1,A2,VDUM
      DIMENSION ATA(10,10),A(6,100),Y(100),X(6),ATY(6),JP(100),KP(100),
     1JPP(100),KPP(100),ENG(50,50),FOBS(30,30,3,3),FCAL(30,30,3,3),
     2FDEL(30,30,3,3),FREQ(100),JDUM(10),VDUM(2),CAL(100),DEL(100)
      CALL NTRAN(20,2,2500,ENG,ISTAT)
      CALL NTRAN(20,22)
      WRITE(6,1)ISTAT
    1 FORMAT(I5,' WORDS TRANSMITTED.')
      N=0
      A1=0.0
      A2=0.0
      DO 99 I=1,6
      DO 99 J=1,6
      DO 99 L=1,100
      A(I,L)=0.0
      ATY(I)=0.0
   99 ATA(I,J)=0.0
      WRITE(6,11)
   11 FORMAT(' ENTER J'', K'', J", K", OBSERVED FREQUENCY.')
  101 N=N+1
      DELSQ=0.0
      READ(5,10)JP(N),KP(N),JPP(N),KPP(N),FREQ(N)
   10 FORMAT()
      IF(JP(N))200,101,101
  200 NTOT=N-1
      DO 210 N=1,NTOT
      A(1,N)=1.0
  210 A(2,N)=JP(N)*(JP(N)+1)
      NUM=2
      WRITE(6,21)
   21 FORMAT(' TO SOLVE FOR A-C, TYPE "1"')
      READ(5,10)JUNK
```

```
      IF(JUNK)215,215,201
  201 DO 211 N=1,NTOT
  211 A(3,N)=KP(N)**2
      NUN=NUN+1
      WRITE(6,22)
   22 FORMAT(' TO SOLVE FOR DK, TYPE "1"')
      READ(5,10)JUNK
      IF(JUNK)215,215,202
  202 DO 212 N=1,NTOT
  212 A(4,N)=KP(N)**4
      NUN=NUN+1
      WRITE(6,23)
   23 FORMAT(' TO SOLVE FOR DJK, TYPE "1"')
      READ(5,10)JUNK
      IF(JUNK)215,215,203
  203 DO 213 N=1,NTOT
  213 A(5,N)=A(2,N)*A(3,N)
      NUN=NUN+1
      WRITE(6,24)
   24 FORMAT(' TO SOLVE FOR DK, TYPE "1"')
      READ(5,10)JUNK
      IF(JUNK)215,215,204
  204 DO 214 N=1,NTOT
  214 A(6,N)=A(2,N)**2
      NUN=NUN+1
  215 DO 216 N=1,NTOT
      L=KPP(N)+1
      J=JPP(N)
  216 Y(N)=FREQ(N)+ENG(J,L)
      DO 250 J=1,6
      DO 250 I=1,6
      A1=0.0D0
      A2=0.0D0
      DO 249 L=1,NTOT
      A1=A1+A(I,L)*A(J,L)
  249 A2=A2+A(I,L)*Y(L)
      ATA(I,J)=A1
  250 ATY(I)=A2
      DO 255 J=1,6
  255 ATA(J,NUN+1)=ATY(J)
      VDUM(1)=4.0
      CALL DGJR(ATA,10,10,NUN,NUN+1,$900,JDUM,VDUM)
      WRITE(6,25)JDUM(1)
   25 FORMAT(I2,' COLUMNS PROCESSED.')
      DO 256 J=1,6
  256 X(J)=ATA(J,NUN+1)
      DO 302 KK=0,10
      K=KK*2+1
      L=K+1
      K10=K+10
      DO 302 J=K,K10
      FCAL(J,L,3,3)=X(1)+X(2)*(J+1)*(J+2)+X(3)*L*L+X(4)*(L**4)+
     1  X(5)*L*L*(J+1)*(J+2)+X(6)*(((J+1)*(J+2))**2)-ENG(J,L)
  302 FCAL(J,L,1,1)=X(1)+X(2)*J*(J-1)+X(3)*((K-1)**2)+X(4)*((K-1)**4)+
     1  X(5)*((K-1)**2)*J*(J-1)+X(6)*((J*(J-1))**2)-ENG(J,L)
      DO 350 N=1,NTOT
      J=JPP(N)
      L=KPP(N)+1
      JD=JP(N)-JPP(N)+2
      KD=KP(N)-KPP(N)+2
```

```
      FOBS(J,L,JD,KD)=FREQ(N)
      FDEL(J,L,JD,KD)=FREQ(N)-FCAL(J,L,JD,KD)
      CAL(N)=FCAL(J,L,JD,KD)
      DEL(N)=FDEL(J,L,JD,KD)
  350 DELSQ=DELSQ+FDEL(J,L,JD,KD)**2
      DELSQ=DELSQ/NTOT
      DELSQ=SQRT(DELSQ)
      WRITE(6,40)(X(J),J=1,6)
   40 FORMAT(' BAND ORIGIN AT',F13.3,' CM-1.'/' B=',F10.6/
     1' A-C=',F10.6/' DK=',F14.12/' DJK=',F14.12/' DJ=',F14.12)
      WRITE(6,41)DELSQ,NTOT
   41 FORMAT(' ROOT MEAN SQUARE DEVIATION=',F8.4,' CM-1 FOR',
     1 I5,' LINES.')
      GO TO 600
  405 WRITE(6,42)
   42 FORMAT(' * * * * * * * * P BRANCH * * * * * * * *')
      WRITE(6,43)
   43 FORMAT('   J''   K''   J"   K"    FREQ CALC   OBSERVED   DIFFERENCE')
      DO 410 KK=1,10
      WRITE(6,44)
   44 FORMAT(1H0)
      L=2*KK
      K10=L+9
      K=L-1
      DO 410 J=K,K10
      JM=J-1
      KM=K-1
  410 WRITE(6,45)JM,KM,J,K,FCAL(J,L,1,1),FOBS(J,L,1,1),FDEL(J,L,1,1)
   45 FORMAT(4I4,3F12.2)
      WRITE(6,46)
   46 FORMAT(' * * * * * * * * R BRANCH * * * * * * * *')
      WRITE(6,44)
      WRITE(6,43)
      DO 420 KK=1,10
      WRITE(6,44)
      L=2*KK
      K10=L+9
      K=L-1
      DO 420 J=K,K10
      JM=J+1
      KM=K+1
  420 WRITE(6,45)JM,KM,J,K,FCAL(J,L,3,3),FOBS(J,L,3,3),FDEL(J,L,3,3)
  500 WRITE(6,51)
   51 FORMAT(' IF YOU WISH TO CHANGE ANY ASSIGNMENTS, TYPE "1"')
      READ(5,10)NOPT
      IF(NOPT-1)505,600,505
  505 WRITE(6,52)
   52 FORMAT(' IF YOU WISH TO ADD ANY ASSIGNMENTS, TYPE "1"')
      READ(5,10)NOPT
      IF(NOPT-1)999,510,999
  510 WRITE(6,11)
      N=NTOT
      DELSQ=0.0
      GO TO 101
  600 WRITE(6,61)
   61 FORMAT(' INDEX   J''   K''   J"   K"    FREQ OBS',
     1 '      FREQ CALC    DIFFERENCE')
      WRITE(6,62)(N,JP(N),KP(N),JPP(N),KPP(N),FREQ(N),
     1  CAL(N),DEL(N),N=1,NTOT)
   62 FORMAT(1X,5I5,3F12.3)
```

```
      WRITE(6,63)
   63 FORMAT(' ENTER INDEX AND REVISED ASSIGNMENTS.')
  605 READ(5,10)N,JQ,KQ,JQQ,KQQ,F
      IF(N)650,650,610
  610 JP(N)=JQ
      KP(N)=KQ
      JPP(N)=JQQ
      KPP(N)=KQQ
      FREQ(N)=F
      GO TO 605
  650 WRITE(6,65)
   65 FORMAT(' TO ADD FURTHER ASSIGNMENTS OR TO RECALCULATE ',
     1   'CONSTANTS, TYPE ¤1¤.')
      READ(5,10)NOPT
      IF(NOPT-1)651,510,651
  651 WRITE(6,66)
   66 FORMAT(' TO PRINT ALL LINE POSITIONS, TYPE ¤1¤.')
      READ(5,10)NOPT
      IF(NOPT-1)652,405,652
  652 WRITE(6,67)
   67 FORMAT(' TO DUMP INTO AN EXTERNAL FILE, TYPE ¤1¤.'/
     1   ' FIRST BE SURE UNIT 24 IS ASSIGNED!')
      READ(5,10)NOPT
      IF(NOPT-1)999,653,999
  653 CALL NTRAN(24,1,3000,FCAL,ISTAT)
      CALL NTRAN(24,22)
      IF(ISTAT)656,656,654
  654 CALL NTRAN(24,1,3000,FOBS,ISTAT)
      CALL NTRAN(24,22)
      IF(ISTAT)656,656,655
  655 CALL NTRAN(24,1,3000,FDEL,ISTAT)
      CALL NTRAN(24,22)
      IF(ISTAT)656,656,657
  656 WRITE(6,68)ISTAT
   68 FORMAT(' ERROR IN TRANSMISSION.  ISTAT =',I3)
      GO TO 651
  657 WRITE(6,69)
   69 FORMAT(' TRANSMISSION COMPLETE.')
      GO TO 999
  900 WRITE(6,91)
   91 FORMAT(' PROGRAM BOMBED OUT IN ROUTINE DGJR.'/
     1 ' TO TRY AGAIN, TYPE ¤1¤.')
      READ(5,10)NOPT
      IF(NOPT-1)999,901,999
  901 N=NTOT+1
      GO TO 200
  999 STOP
      END
```

The ground state rotational term values were calculated using the rotational constants of Kivelson (35) for SO_2^{16} and of Van Riet, et al. (49), for SO_2^{18}. These constants are listed in Table 4.

The method of computation has been described by J. T. Murray (50), and the computer program used for these calculations is described in his doctoral dissertation. The technique involves computing the eigenvalues F_τ^J of the matrix $\langle H' \rangle$ of the reduced Hamiltonian

$$H' = P_a^2 + \frac{2B-A-C}{A-C} (P_b^2 - P_c^2)$$

whose elements are given by the relations

$$\langle J,K|H'|J,K\rangle = \tfrac{1}{2}(\kappa-1)J(J+1) + \tfrac{1}{2}(3-\kappa)K^2$$

and

$$\langle J,K|H'|J,K+2\rangle = \langle J,K+2|H'|J,K\rangle$$

$$= -\tfrac{1}{2}(\kappa+1)\left\{\left[\frac{J(J+1)}{4} - K(K+1)\right]\left[J(J+1) - (K+1)(K+2)\right]\right\}^{\frac{1}{2}} .$$

Here, A, B, and C are the principal moments of inertia and P_a, P_b, and P_c are the components of the total angular momentum along the principal axes. The parameter κ is defined as

$$\kappa = \frac{2B-A-C}{A-C}$$

Table 4. Ground State Rotational Constants

	SO_2^{16}	SO_2^{18}
A	60778.79 MHz	57384.53 MHz
B	10318.10 MHz	9170.35 MHz
C	8799.96 MHz	7889.60 MHz
D_J	2.06×10^{-7} cm^{-1}	(a)
D_K	8.54×10^{-5} cm^{-1}	(a)
D_{JK}	-3.74×10^{-6} cm^{-1}	(a)

[a]Not used in this calculation.

and τ is an integral index running from J (for the highest energy term value of a given J-manifold) to -J (for the term value of lowest energy).

The rotational energies are then given by

$$E^J_\tau = \tfrac{1}{2}(A+C)J(J+1) + \tfrac{1}{2}(A-C)F^J_\tau$$

The computer program was modified by the author to include the terms in centrifugal distortion appropriate to a prolate symmetric rotor. This modification proved of little value, since the accuracy to which high-K sub-bands could be reproduced was limited by the model for the excited state.

STORE is a program which reads rotational term values, along with appropriate values of J and τ, and stores them in a disc file in a form suitable for retrieval by other programs (such as FIT). Unit 20 must be assigned for the output of this program.

```
      DIMENSION A(50,50)
      READ(5,11)JOKER
   11 FORMAT(I3)
  101 READ(5,12,END=200)J,I,DATIN
   12 FORMAT(2I5,F25.6 )
      IF(JOKER)102,999,103
  102 K=(I+J+1)*.5
      L=K+1
      A(J,L)=DATIN
      WRITE(6,12)J,K,A(J,L)
  103 JOKER=JOKER*(-1)
      GO TO 101
  200 CALL NTRAN(20,1,2500,A,ISTAT)
      CALL NTRAN(20,22)
      WRITE(6,21)ISTAT
   21 FORMAT(I5, 19H WORDS TRANSMITTED.     )
  999 STOP
      END
```

SPEC calculates the frequency of transition from an asymmetric rotor ground electronic state to a linear or nearly linear excited state, given the band origin, rotational constants, and ground state rotational term values. The method of computation is essentially the same as that used in FIT.

```
      DIMENSION AA(50,50)
   11 FORMAT(' ENTER A-C, B, NU ZERO, DK, DJK, DJ')
   12 FORMAT()
   13 FORMAT(' ENTER SELECTION RULES ON J AND K.')
   14 FORMAT(I5,' WORDS TRANSMITTED')
   20 FORMAT('  J  K  FREQUENCY CALCULATED')
   21 FORMAT(2I3,F12.3)
      CALL NTRAN(20,3,2500,AA,ISTAT)
      CALL NTRAN(20,22)
      WRITE(6,14)ISTAT
      WRITE(6,11)
      READ(5,12)A,B,Z,DK,DJK,DJ
      WRITE(6,13)
      READ(5,12)JDEL,KDEL
      WRITE(6,20)
      DO 200 KK=0,10
      K=KK*2
      K1=K+6
      DO 200 J=K,K1
      F=Z+A*K*K+B*J*(J+1)+DJK*((J*(J+1)))*K**2+DJ*J*J*((J+1)**2)
     1 +DK*(K**4)
      J1=J-JDEL
      L=K-KDEL+1
      F=F-AA(J1,L)
  200 WRITE(6,21)J,K,F
      STOP
      END
```

SPCALC computes the transition frequencies for the molecule as in SPEC, and in addition calculates intensities of absorption lines using the Honl-London formulas (53). Output is plotted using a Calcomp plotter.

```
      DIMENSION SPC(10000),F(50,50),RECORD(12),IBUF(1400)
      DIMENSION S1(2500),S2(2500),S3(2500),S4(2500)
      EQUIVALENCE (S1,SPC),(S2,SPC(2501)),(S3,SPC(5001)),(S4,SPC(7501))
      CALL PLOTS(IBUF,1000,22)
      CALL CHARGE
      CALL PLOTMX(50.)
      CALL PLOT(0.0,-3.0,-3)
      CALL NTRAN(20,2,2500,F,ISTAT)
      CALL NTRAN(20,22)
      WRITE(6,10)ISTAT
   10 FORMAT(I5,' WORDS TRANSMITTED.')
      WRITE(6,11)
   11 FORMAT(' ENTER ONE LINE PROBLEM IDENTIFICATION')
      READ(5,6)(RECORD(I),I=1,12)
      CALL SYMBOL(0.0,0.5,.14,RECORD,90.,72)
      CALL PLOT(1.5,0.2,-3)
    6 FORMAT(12A6)
C     PLOT LEGEND
      WRITE(6,12)
   12 FORMAT(' ENTER BAND ORIGIN, A-B, AND B.')
      READ(5,5)ORIGIN,AMB,B
    5 FORMAT( )
      WRITE(6,13)
   13 FORMAT(' ENTER C, KT')
      READ(5,5)C,TK
      WRITE(6,14)
   14 FORMAT(' ENTER V''; THEN 1 IF K'' IS ODD, ZERO IF EVEN.')
      READ(5,5)NV,JOKER
      KKMAX=(NV-JOKER)/2
```

```
      WRITE(6,15)
   15 FORMAT(' ENTER STARTING POINT OF PLOT.')
      READ(5,5)ZERO
C     (P)P BRANCH   (J-1,K-1<--J,K)
      JSYM=1
      DO 310 KK=0,KKMAX
      K=KK*2+JOKER+1
      DO 310 J=K,29
      IF(K-1)303,303,304
  303 JSYM=-JSYM
      IF(JSYM)310,304,304
  304 FREQ=AMB*((K-1)**2)+B*(J-1)*J+ORIGIN-F(J,K+1)
      INDX=(ZERO-FREQ)*40.
      IF(INDX)990,305,305
  305 IF(10000-INDX)990,306,306
  306 CONTINUE
      G=2.*J+1.
      AKJ=(1.*(J+K)*(J+K-1))/(J*(2*J+1))
      E=-F(J,K+1)/TK
      SPC(INDX)=SPC(INDX)+C*FREQ*AKJ*G*(EXP(E))
  310 CONTINUE
      JSYM=1
C     (P)Q BRANCH   (J,K-1<--J,K)
      DO 320 KK=0,KKMAX
      K=KK*2+JOKER+1
      DO 320 J=K,29
C     K'=0 HAS ONLY ODD J' LEVELS ALLOWED
      IF(K-1)313,313,314
  313 JSYM=-JSYM
      IF(JSYM)314,314,320
  314 FREQ=AMB*((K-1)**2)+B*J*(J+1)+ORIGIN-F(J,K+1)
      INDX=(ZERO-FREQ)*40.
      G=2.*J+1.
      AKJ=(1.*(J-K+1)*(J+K))/(J*(J+1))
      E=-F(J,K+1)/TK
      SPC(INDX)=SPC(INDX)+C*FREQ*AKJ*G*(EXP(E))
  320 CONTINUE
      JSYM=1
C     (P)R BRANCH   (K-1,J+1<--K,J)
      DO 330 KK=0,KKMAX
      K=KK*2+JOKER+1
      DO 330 J=K,29
      IF(K-1)323,323,324
  323 JSYM=-JSYM
      IF(JSYM)330,324,324
  324 FREQ=(AMB*((K-1)**2)+B*(J+1)*(J+2))+ORIGIN-F(J,K+1)
      INDX=(ZERO-FREQ)*40.
      G=2.*J+1.
      AKJ=(1.*(J-K+2)*(J-K+1))/((J+1)*(2*J+1))
      E=-F(J,K+1)/TK
      SPC(INDX)=SPC(INDX)+C*FREQ*AKJ*G*(EXP(E))
  330 CONTINUE
      JSYM=-1
C     (R)P BRANCH   (J-1,K+1<--J,K)
      DO 340 KK=0,KKMAX
      K=KK*2+JOKER-1
      JJ=K+2
      DO 340 J=JJ,29
      IF(K)340,331,332
  331 JSYM=JSYM*(-1)
```

```
      IF(JSYM)340,332,332
  332 FREQ=AMB*((K+1)**2)+B*(J+1)*(J+2)+ORIGIN-F(J,K+1)
      INDX=(ZERO-FREQ)*40
      G=2.*J+1.
      AKJ=(1.*(J-K-1)*(J-K))/(J*(2*J+1))
      E=-F(J,K+1)/TK
      SPC(INDX)=SPC(INDX)+C*FREQ*AKJ*G*(EXP(E))
  340 CONTINUE
      JSYM=1
C     (R)Q BRANCH   (J,K+1<--J,K)
      DO 350 KK=0,KKMAX
      K=KK*2+JOKER-1
      JJ=K+1
      DO 350 J=JJ,29
      IF(K)350,341,342
  341 JSYM=JSYM*(-1)
      IF(JSYM)350,342,342
  342 FREQ=AMB*((K+1)**2)+B*(J+1)*(J+2)+ORIGIN-F(J,K+1)
      INDX=(ZERO-FREQ)*40
      G=2.*J+1.
      AKJ=(1.*(J+K+1)*(J-K))/(J*(J+1))
      E=-F(J,K+1)/TK
      SPC(INDX)=SPC(INDX)+C*FREQ*AKJ*G*(EXP(E))
  350 CONTINUE
      JSYM=-1
C     (R)R BRANCH    (J+1,K+1<--J,K)
      DO 360 KK=0,KKMAX
      K=KK*2+JOKER-1
      DO 360 J=K,29
      IF(K)360,351,352
  351 JSYM=JSYM*(-1)
      IF(JSYM)360,352,352
  352 FREQ=AMB*((K+1)**2)+B*(J+1)*(J+2)+ORIGIN-F(J,K+1)
      INDX=(ZERO-FREQ)*40
      G=2.*J+1.
      AKJ=(1.*(J+K+2)*(J+K+1))/((J+1)*(2*J+1))
      E=-F(J,K+1)/TK
      SPC(INDX)=SPC(INDX)+C*FREQ*AKJ*G*(EXP(E))
  360 CONTINUE
      DO 410 IDUM=1,5
      CALL DAMP(S1,2500)
      CALL DAMP(S2,2500)
      CALL DAMP(S3,2500)
  410 CALL DAMP(S4,2500)
      DO 420 I=1,10000
      X=(1.*I)/400.
      Y=SPC(I)+4.
      ABSTOT=ABSTOT+SPC(I)
  420 CALL PLOT(X,Y,2)
      CALL AXIS(0.,3.0,15HFREQUENCY, CM-1 ,-15,30.,0.0,ZERO,-10.)
      CALL TIC(0.0,30.0)
      CALL PLOT(30.0,0.0,999)
      WRITE(6,50)ABSTOT
   50 FORMAT(F15.0,' IS THE INTEGRATED INTENSITY, WITHOUT THE '/
     1 ' FRANCK-CONDON FACTOR.')
      CALL EXIT
  990 WRITE(6,99)INDX,FREQ,J,K
   99 FORMAT(' ERROR. INDX, FREQ, J, AND K ARE',I6,F12.3,2I6)
      END
```

MRSPEC calculates line positions and intensities for the magnetic rotation spectrum of SO_2, using the approximation that only field-induced mixing is important. The "B" terms are calculated according to the formulas of Buckingham and Stephens (54) assuming that Zeeman splitting of states with different values of M_J is zero.

```
      DIMENSION SRM(10000),A(12),RB(12)
      DIMENSION EG(50,50),PHI(10000),THETA(10000),IBUF(1000),RECORD(24)
      EQUIVALENCE (A,RECORD),(RB,RECORD(13))
      EQUIVALENCE(SRM,PHI)
      CALL PLOTS(IBUF,1000,22)
      CALL CHARGE
      CALL PLOTMX(50.)
      CALL PLOT(0.0,-3.0,-3)
      CALL NTRAN(20,2,2500,EG,ISTAT)
      CALL NTRAN(20,22)
      WRITE(6,10)ISTAT
   10 FORMAT(I5,' WORDS TRANSMITTED.'/' BE SURE UNITS 24 AND ',
     1'25 ARE ASSIGNED!')
      WRITE(6,11)
   11 FORMAT(' ENTER TWO LINES PROBLEM IDENTIFICATION')
      READ(5,6)(RECORD(I),I=1,24)
      CALL SYMBOL(0.0,0.5,.14,A,90.,72)
      CALL PLOT(1.0,-.5,-3)
      CALL SYMBOL(0.0,0.5,.14,RB,90.,72)
      CALL PLOT(1.0,-.5,-3)
    6 FORMAT(12A6)
C     PLOT LEGEND
      WRITE(6,12)
   12 FORMAT(' ENTER BAND ORIGIN, A-B, AND B.')
      READ(5,5)ORIGIN,AMB,B
    5 FORMAT( )
      WRITE(6,13)
   13 FORMAT(' ENTER BETA 1, BETA 1'', BETA 2, GAMMA, AND H.')
      READ(5,5)BET1,BET11,BET2,GAMMA,H
      WRITE(6,14)
   14 FORMAT(' ENTER V'';  THEN 1 IF K'' IS ODD, ZERO IF EVEN.')
      READ(5,5)NV,JOKER
      KMAX=(NV-JOKER)/2
      WRITE(6,15)
```

```
   15 FORMAT(' ENTER STARTING POINT OF PLOT.')
      READ(5,5)ZERO
C     (P)P+ BRANCH    (J-1,K-1,M+1<--J,K,M)
      JSYM=1
      BETA=BET1
  301 DO 310 KK=0,KKMAX
      K=KK*2+JOKER+1
      IF(K-1-NV)306,305,311
  305 BETA=BET11
  306 JM=29
      DO 310 J=K,JM
      IF(K-1)307,307,308
  307 JSYM=-JSYM
      IF(JSYM)310,310,308
  308 FREQ=AMB*((K-1)**2)+B*(J-1)*J+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=-1*J
      J2=J-2
      IF(J2-NJ)310,3081,3081
 3081 CONTINUE
      DO 309 M=NJ,J2
      B1=(BETA*(J*J-K*K)*(J*J-M*M)*(J+K-1)*(J-M-1))/(16*J*J*J*(J-1)
     1*(2*J-1)*(2*J+1))
      B2=(BETA*(J-M)*(J-M-1)*(J+K)*(J+K-1)*K*M)/(16*J*J*J*(J+1)*
     1 (2*J-1)*(2*J+1))
      B3=(BET2*(J+K)*(J+K-1)*(J-M)*(J-M-1)*(K-1)*(M+1))/(16*J*J*J*(J-1)*
     1 (2*J-1)*(2*J+1))
      B4=(BET2*(J+K)*(J*J-(K-1)**2)*(J-M)*(J*J-(M+1)**2))/(16*(J+1)*
     1 J*J*J*(2*J-1)*(2*J+1))
      BTERM=B2-B1+B3-B4
      BTERM=BTERM*BOL
  309 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  310 CONTINUE
  311 BETA=BET1
      WRITE(6,31)
   31 FORMAT(' PASSING LABEL 310')
C     (P)P- BRANCH   (J-1,K-1,M-1<--J,K,M)
  321 DO 330 KK=0,KKMAX
      JSYM=1
      K=KK*2+JOKER+1
      IF(K-1-NV)326,325,331
  325 BETA=BET11
  326 JM=29
      DO 330 J=K,JM
      IF(K-1)327,327,328
  327 JSYM=-JSYM
      IF(JSYM)330,330,328
  328 FREQ=AMB*((K-1)**2)+B*J*(J-1)+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=2-J
      IF(J-NJ)330,3281,3281
 3281 CONTINUE
      DO 329 M=NJ,J
      B1=(BETA*(J*J-K*K)*(J*J-M*M)*(J+K-1)*(J+M-1))/(16*J*J*J*(J-1)*
     1 (2*J-1)*(2*J+1))
      B2=(BETA*K*M*(J+K)*(J+K-1)*(J+M)*(J+M-1))/(16*J*J*J*(J+1)*
     1 (2*J-1)*(2*J+1))
      B3=(BET2*(J+K)*(J+K-1)*(J+M)*(J+M-1)*(M-1)*(K-1))/(16*J*J*J*(J-1)*
```

```
     1(4*J*J-1))
      B4=(BET2*(J+K)*(J+M)*(J*J-((K-1)**2))*(J*J-((M-1)**2)))/(
     1 16*J*J*J*(J+1)*(2*J-1)*(2*J+1))
      BTERM=-B1-B2-B3-B4
      BTERM=BTERM*BOL
  329 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  330 CONTINUE
      WRITE(6,33)
   33 FORMAT(' PASSING LABEL 330')
  331 BETA=BET1
C     (P)Q- BRANCH    (J,K-1,M-1<--J,K,M)
      JSYM=-1
      DO 350 KK=0,KKMAX
      K=KK*2+JOKER+1
      IF(K-1-NV)346,345,351
  345 BETA=BET11
  346 JM=29
      DO 350 J=K,JM
      IF(K-1)347,347,348
  347 JSYM=-JSYM
      IF(JSYM)350,350,348
  348 FREQ=AMB*((K-1)**2)+B*J*(J-1)+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=1-J
      IF(J-NJ)350,3481,3481
 3481 CONTINUE
      DO 349 M=NJ,J
      B1=(BETA*(J+K)*(J-K+1)*(J+M)*(J-M+1)*K*M)/(16*J*J*J*((J+1)**3))
      B2=(BETA*(J+K)*(J+M)*(((J+1)**2)-M*M)*(((J+1)**2)-K*K))/(16*
     1 J*J*((J+1)**2)*(2*J+1)*(2*J+3))
      B3=(BETA*(J-K+1)*(J-M+1)*(J*J-K*K)*(J*J-M*M))/(16*J*J*J*
     1   (J+1)*(4*J*J-1))
      B4=(BET2*(J+K)*(J+M)*(J-K+1)*(J-M+1)*(K-1)*(M-1))/
     1 (16*J*J*J*((J+1)**3))
      B5=(BET2*(J-K+1)*(J-M+1)*(((J+1)**2)-((K-1)**2))*(((J+1)**2)
     1 -((M-1)**2)))/(16*J*((J+1)**3)*(2*J+1)*(2*J+3))
      B6=(BET2*(J+K)*(J+M)*(J*J-((K-1)**2))*(J*J-((M-1)**2)))/
     1 (16*J*J*J*(J+1)*(4*J*J-1))
      BTERM=-(B1+B2+B3+B4+B5+B6)*BOL
  349 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  350 CONTINUE
  351 BETA=BET1
      WRITE(6,35)
   35 FORMAT(' PASSING LABEL 350')
C     (P)Q+ BRANCH     (J,K-1,M+1<--J,K,M)
      JSYM=-1
      DO 370 KK=0,KKMAX
      K=KK*2+JOKER+1
      IF(K-1-NV)366,365,371
  365 BETA=BET11
  366 JM=29
      DO 370 J=K,JM
      IF(K-1)367,367,368
  367 JSYM=-JSYM
      IF(JSYM)370,370,368
  368 FREQ=AMB*((K-1)**2)+B*J*(J-1)+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=-1*J
```

```
      J1=J-1
      IF(J1-NJ)370,3681,3681
 3681 CONTINUE
      DO 369 M=NJ,J1
      B1=(BETA*(J+K)*(J-K+1)*(J-M)*(J+M+1)*M*K)/(16*J*J*J*((J+1)**3))
      B2=(BETA*(J+K)*(J-M)*(((J+1)**2)-K*K)*(((J+1)**2)-M*M))/(
     1 16*J*((J+1)**3)*(2*J+1)*(2*J+3))
      B3=(BETA*(J*J-K*K)*(J*J-M*M)*(J-K+1)*(J+M+1))/(
     1 16*J*J*J*(J+1)*(4*J*J-1))
      B4=(BET2*(J+K)*(J-M)*(J-K+1)*(J+M+1)*(K-1)*(M+1))/(16*
     1   J*J*J*((J+1)**3))
      B5=(BET2*(((J+1)**2)-((K-1)**2))*(J-K+1)*(((J+1)**2)-((M+1)
     1 **2))*(J+M+1))/(16*J*((J+1)**3)*(2*J+1)*(2*J+3))
      B6=(BET2*(J*J-((K-1)**2))*(J+K)*(J*J-((M+1)**2))*(J-M))/(
     1 16*J*J*J*(J+1)*(4*J*J-1))
      BTERM=(B1-B2-B3+B4-B5-B6)*BOL
  369 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  370 CONTINUE
  371 BETA=BET1
      WRITE(6,37)
   37 FORMAT(' PASSING LABEL 370')
C     (P)R- BRANCH    (J+1,K-1,M-1<--J,K,M)
      JSYM=1
      DO 390 KK=0,KKMAX
      K=KK*2+JOKER+1
      IF(K-1-NV)386,385,391
  385 BETA=BET11
  386 JM=29
      DO 390 J=K,JM
      IF(K-1)387,387,388
  387 JSYM=-JSYM
      IF(JSYM)390,390,388
  388 FREQ=AMB*((K-1)**2)+B*(J+1)*(J+2)+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=-J
      DO 389 M=NJ,J
      B1=(BETA*(J-K+1)*(J-K+2)*(J-M+1)*(J-M+2)*K*M)/(16*J*((J+1)**3)*
     1(2*J+1)*(2*J+3))
      B2=(BETA*(((J+1)**2)-K*K)*(((J+1)**2)-M*M)*(J-K+2)*(J-M+2))
     1 /(16*((J+1)**3)*(J+2)*(2*J+1)*(2*J+3))
      B3=(BET2*(J-K+1)*(J-K+2)*(J-M+1)*(J-M+2)*(K-1)*(M-1))/
     1 (16*((J+1)**3)*(J+2)*(2*J+1)*(2*J+3))
      B4=(BET2*(J-K+1)*(J-M+1)*(((J+1)**2)-((K-1)**2))*(((J+1)**2
     1)-((M-1**2))))/(16*J*((J+1)**3)*(2*J+1)*(2*J+3))
      BTERM=(-B1-B2-B3-B4)*BOL
  389 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  390 CONTINUE
  391 BETA=BET1
      WRITE(6,39)
   39 FORMAT(' PASSING LABEL 391')
C     (P)R+ BRANCH    (J+1,K-1,M+1<--J,K,M)
      JSYM=1
      DO 410 KK=0,KKMAX
      K=KK*2+JOKER+1
      IF(K-1-NV)406,405,411
  405 BETA=BET11
  406 JM=29
      DO 410 J=K,JM
      IF(K-1)407,407,408
```

```
  407 JSYM=-JSYM
      IF(JSYM)410,410,408
  408 FREQ=AMB*((K-1)**2)+B*(J+1)*(J+2)+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=-J
      DO 409 M=NJ,J
      DNOM=16*((J+1)**3)*(2*J+1)*(2*J+3)
      B1=(BETA*(((J+1)**2)-M*M)*(((J+1)**2)-K*K)*(J+M+2)*(J-K+2))/
     1(DNOM*(J+2))
      B2=(BETA*(J+M+1)*(J+M+2)*(J-K+1)*(J-K+2)*M*K)/(DNOM*J)
      B3=(BET2*(J+M+1)*(J+M+2)*(J-K+1)*(J-K+2)*(K-1)*(M+1))/((J+2)*
     1 DNOM)
      B4=(BET2*(J-K+1)*(((J+1)**2)-((K-1)**2))*(((J+1)**2)-((M+1)**2))*
     1(J+M+1))/(DNOM*J)
      BTERM=(-B1+B2+B3-B4)*BOL
  409 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  410 CONTINUE
  411 BETA=BET1
      WRITE(6,41)
   41 FORMAT(' PASSING LABEL 410')
      JSYM=-1
C     (R)P- BRANCH      (J-1,K+1,M-1<--J,K,M)
      DO 431 KK=0,KKMAX
      K=KK*2+JOKER-1
      JJ=K+2
      JM=29
      DO 431 J=JJ,JM
      IF(K)431,412,413
  412 JSYM=-JSYM
      IF(JSYM)431,413,413
  413 FREQ=AMB*((K+1)**2)+B*J*(J-1)+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=2-J
      DO 430 M=NJ,J
      DNOM=16*J*J*J*(4*J*J-1)
      B1=(BETA*(J*J-K*K)*(J*J-M*M)*(J+M-1)*(J-K-1))/((J-1)*DNOM)
      B2=(BETA*(J-K)*(J-K-1)*(J+M)*(J+M-1)*K*M)/(DNOM*(J+1))
      B3=(BET2*(J+M)*(J+M-1)*(J-K)*(J-K-1)*(K+1)*(M-1))/(DNOM*(J-1))
      B4=(BET2*(J+M)*(J*J-((M-1)**2))*(J-K)*(J*J-((K+1)**2)))/
     1(DNOM*(J+1))
      BTERM=(B1-B2-B3+B4)*BOL
  430 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  431 CONTINUE
      WRITE(6,43)
   43 FORMAT(' PASSING LABEL 430')
      JSYM=-1
C     (R)P+ BRANCH   (J-1,K+1,M+1<--J,K,M)
      DO 451 KK=0,KKMAX
      K=KK*2+JOKER-1
      JJ=K+2
      DO 451 J=JJ,29
      IF(K)451,432,433
  432 JSYM=-JSYM
      IF(JSYM)451,433,433
  433 FREQ=AMB*((K+1)**2)+B*(J-1)*J+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=-J
```

```
      J2=J-2
      DO 450 M=NJ,J2
      DNOM=J*J*J+16*(4*J*J-1)
      B1=(BETA*(J-K)*(J-K-1)*(J-M)*(J-M-1)*K*M)/((J+1)*DNOM)
      B2=(BETA*(J*J-K*K)*(J-K-1)*(J*J-M*M)*(J-M-1))/((J-1)*DNOM)
      B3=(BET2*(J-K)*(J-M)*(J*J-((K+1)**2))*(J*J-((M+1)**2)))/
     1((J+1)*DNOM)
      B4=(BET2*(J-K)*(J-K-1)*(J-M)*(J-M-1)*(K+1)*(M+1))/((J-1)*DNOM)
      BTERM=(B1+B2+B3+B4)*BOL
  450 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  451 CONTINUE
      WRITE(6,45)
   45 FORMAT(' PASSING LABEL 450')
      JSYM=1
C     (R)Q+      (J,K+1,M+1<--J,K,M)
      DO 471 KK=0,KKMAX
      K=KK*2+JOKER-1
      JJ=K+1
      DO 471 J=JJ,29
      IF(K)471,452,453
  452 JSYM=-JSYM
      IF(JSYM)471,453,453
  453 E=EG(J,K+1)
      FREQ=AMB*((K+1)**2)+B*J*(J+1)+ORIGIN-E
      BOL=EXP(-E/140.)
      NJ=1-J
      DO 470 M=NJ,J
      D1=16*J*J*J*((J+1)**3)
      D2=16*J*((J+1)**3)*(2*J+1)*(2*J+3)
      D3=16*J*J*J*(J+1)*(4*J*J-1)
      B1=(BETA*(J-K)*(J+K+1)*(J-M)*(J+M+1)*K*M)/D1
      B2=(BETA*(J-K)*(J-M)*(((J+1)**2)-K*K)*(((J+1)**2)-M*M))/D2
      B3=(BETA*(J*J-K*K)*(J+K+1)*(J*J-M*M)*(J+M+1))/D3
      B4=(BET2*(J-K)*(J+K+1)*(J-M)*(J+M+1)*(K+1)*(M+1))/D1
      B5=(BET2*(J+K+1)*(J+M+1)*(((J+1)**2)-((K+1)**2))*(((J+1)**2)-((M
     1+1)**2)))/D2
      B6=(BET2*(J-K)*(J-M)*(J*J-((K+1)**2))*(J*J-((M+1)**2)))/D3
      BTERM=(B1+B2+B3+B4+B5+B6)*BOL
  470 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  471 CONTINUE
      WRITE(6,47)
   47 FORMAT('PASSING LABEL 470')
      JSYM=1
C     (R)Q- BRANCH     (J,K+1,M-1<--J,K,M)
      DO 491 KK=0,KKMAX
      K=KK*2+JOKER-1
      JJ=K+1
      DO 491 J=JJ,29
      IF(K)491,472,473
  472 JSYM=-JSYM
      IF(JSYM)491,473,473
  473 FREQ=AMB*((K+1)**2)+B*J*(J+1)+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=-J
      J1=J-1
      DO 490 M=NJ,J1
      D1=16*J*J*J*((J+1)**3)
      D2=16*J*((J+1)**3)*(2*J+1)*(2*J+3)
      D3=16*J*J*J*(J+1)*(4*J*J-1)
```

```
      B1=(BETA*(J-K)*(J+M)*(J+K+1)*(J-M+1)*K*M)/D1
      B2=(BETA*(J-K)*(J+M)*(((J+1)**2)-K*K)+(((J+1)**2)-M*M))/D2
      B3=(BETA*(J*J-M*M)*(J*J-K*K)*(J-M+1)*(J+K+1))/D3
      B4=(BET2*(J+M)*(J-M+1)*(J-K)*(J+K+1)*(K+1)*(M-1))/D1
      B5=(BETA*(((J+1)**2)-((M-1)**2))*(J-M+1)*(((J+1)**2)-((K+1)**2))*
     1(J+K+1))/D2
      B6=(BET2*(J*J-((M-1)**2))*(J+M)*(J*J-((K+1)**2))*(J-K))/D3
      BTERM=(-B1+B2+B3-B4+B5+B6)*BOL
  490 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  491 CONTINUE
      WRITE(6,49)
   49 FORMAT(' PASSING LABEL 490')
      JSYM=-1
C     (R)R- BRANCH      (J+1,K+1,M-1<--J,K,M)
      DO 511 KK=0,KKMAX
      K=KK*2+JOKER-1
      DO 511 J=K,29
      IF(K)511,492,493
  492 JSYM=-JSYM
      IF(JSYM)511,493,493
  493 FREQ=AMB*((K+1)**2)+B*(J+1)*(J+2)+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=-J
      DO 510 M=NJ,J
      DNOM=16*((J+1)**3)*(2*J+1)*(2*J+3)
      B1=(BETA*(((J+1)**2)-K*K)*(((J+1)**2)-M*M)*(J+K+2)*(J-M+2))/
     1((J+2)*DNOM)
      IF(J)494,494,495
  494 B2=0.0
      GO TO 496
  495 B2=(BETA*(J+K+1)*(J+K+2)*(J-M+1)*(J-M+2)*M*K)/(J*DNOM)
  496 B3=(BET2*(J+K+1)*(J+K+2)*(J-M+1)*(J-M+2)*(M-1)*(K+1))/((J+2)*DNOM)
      IF(J)497,497,498
  497 B4=0.
      GO TO 499
  498 B4=(BET2*(((J+1)**2)-((K+1)**2))*(((J+1)**2)-((M-1)**2))*(J+K+1)*(
     1J-M+1))/(J*DNOM)
  499 BTERM=(B1-B2-B3+B4)*BOL
  510 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  511 CONTINUE
      WRITE(6,51)
   51 FORMAT(' PASSING LABEL 510')
      JSYM=-1
C     (R)R+ BRANCH       (J+1,K+1,M+1<--J,K,M)
      DO 531 KK=0,KKMAX
      K=KK*2+JOKER-1
      DO 531 J=K,29
      IF(K)531,512,513
  512 JSYM=-JSYM
      IF(JSYM) 531,513,513
  513 FREQ=AMB*((K+1)**2)+B*(J+1)*(J+2)+ORIGIN-EG(J,K+1)
      E=EG(J,K+1)
      BOL=EXP(-E/140.)
      NJ=-J
      DO 530 M=NJ,J
      DNOM=16*((J+1)**3)*(2*J+1)*(2*J+3)
      B1=(BETA*(((J+1)**2)-K*K)*(((J+1)**2)-M*M)*(J+K+2)*(J+M+2))/(
     1(J+2)*DNOM)
      IF(J)514,514,515
```

```
  514 B2=0.0
      GO TO 516
  515 B2=(BETA*(J+K+1)*(J+K+2)*(J+M+1)*(J+M+2)*K*M)/(J*DNOM)
  516 B3=(BET2*(J+K+1)*(J+K+2)*(J+M+1)*(J+M+2)*(K+1)*(M+1))/((J+2)
     1*DNOM)
      IF(J)517,517,518
  517 B4=0.0
      GO TO 519
  518 B4=(BET2*(J+K+1)*(J+M+1)*(((J+1)**2)-((M+1)**2))*(((J+1)**2)-
     1((M+1)**2)))/(J*DNOM)
  519 BTERM=(B1+B2+B3+B4)*BOL
  530 CALL ENTER(FREQ,BTERM,GAMMA,PHI,THETA,ZERO)
  531 CONTINUE
      WRITE(6,53)
   53 FORMAT(' PASSING LABEL 530')
      CALL NTRAN(24,1,10000,PHI,ISTAT)
      CALL NTRAN(24,22)
      WRITE(6,60)ISTAT
   60 FORMAT(I7,' WORDS TRANSMITTED')
      CALL NTRAN(25,1,10000,THETA,ISTAT)
      CALL NTRAN(25,22)
      WRITE(6,60)ISTAT
      DO 620 I=1,10000
      SRM(I)=PHI(I)**2+THETA(I)**2
      IF(SRM(I)-SMAX)602,602,601
  601 SMAX=SRM(I)
  602 CONTINUE
  620 CONTINUE
      WRITE(6,61)SMAX
   61 FORMAT(' MAXIMUM MRS INTENSITY IS',E12.6)
      WRITE(6,62)
   62 FORMAT(' ENTER MRS PLOT SCALE FACTOR.')
      READ(5,5)YSC
      DO 700 I=1,10000
      X=(1.*I)/400.
      Y=SRM(I)*YSC/4.
      SRMTOT=SRMTOT+SRM(I)
  700 CALL PLOT(X,Y,2)
      CALL AXIS(0.,3.0,15HFREQUENCY, CM-1 ,-15,30.0,0.0,ZERO,-10.)
      CALL TIC(0.0,30.0)
      CALL PLOT(30.,0.,999)
      SRMTOT=SRMTOT*YSC
      WRITE(6,71)SRMTOT
   71 FORMAT(' INTEGRATED SPECTRUM INTENSITY IS',F12.0)
      STOP
      END
```

```
      SUBROUTINE ENTER(FREQ,B,GAMMA,PHI,THETA,ZERO)
      DIMENSION PHI(10000),THETA(10000)
      X=((ZERO-FREQ)*40.)
      INDX=X
      I1=INDX-30
      I2=INDX+30
      IF(I1)999,999,110
  110 IF(10000-I2)999,999,111
  111 DO 200 IX=I1,I2
      F=ZERO-(IX*1.)/40.
      THETA(IX)=(F*F*F*GAMMA*B/(((FREQ**2)-F*F)**2+F*F*(GAMMA**2)))+
     1 THETA(IX)
      PHI(IX)=(F*F*(FREQ**2-F**2)*B/(((FREQ**2)-F*F)**2+F*F*(GAMMA**2))
     1)+PHI(IX)
  200 CONTINUE
      GO TO 1000
  999 WRITE(6,99)FREQ
   99 FORMAT(' WARNING:  CALCULATED FREQUENCY EXCEEDS PLOT LIMITS.',
     1F15.6)
 1000 RETURN
      END
```

RENNER computes the vibronic rotational energy of a triatomic molecule according to the second-order perturbation formulas of Merer and Travis (Eq. (14)). It also computes an effective value of A according to Eq. (20) and compares the exact energies computed by the perturbation with those obtained by the symmetric top approximation. This program enabled us to determine that, for $K \leq v_2 - 5$, the symmetric top approximation is an adequate representation of rotational term values for a variety of choices of η, ω_2, and g_{22}. Because of the fundamental objections to the appropriateness of the perturbation approach of Merer and Travis, as discussed in Chapter IV, an attempt to determine precise values of g_{22} and η for SO_2 was not deemed worthwhile.

```
      INTEGER V
      WRITE (6,10)
   10 FORMAT(' ENTER ETA, G, V, OMEGA')
      READ(5,5)E,G,V,W
    5 FORMAT()
      AE=ABS(E)
      E0=-3*AE*(V*V+2*V)-(E*E/W)*17*V*(V+1)*(V+2)+4*G
      WRITE(6,11)
   11 FORMAT('  K   PERTURBATION   SYM TOP      DIFF')
      DO 200 K=0,V
      K2=K*K
      A=-(8*G*G-9*E*E*(V*V+2*V+2))/(3*E*V*(V+2))
      A=A-(3*E*E/W)*(V+1)
      A=A+G
      A=A-(E*G/W)*(V+1)*((34.*V*(V+2))/3-48.)/(V*V+2)
      EST=A*K2+E0
      AMS=64*K2*G*G+36*E*E*(V*V-K2)*((V+2)**2-K2)
      ER=-.5*(SQRT(AMS))
      ER=ER-(E*E/W)*(V+1)*(17*V*(V+2)+3*K2)+G*(K2+4)
      ER=ER+(E*E/W)*(V+1)*K2*(-4*G)*(17*V*(V+2)-15*K2+72)/(SQRT(AMS))
      ED=ER-EST
  200 WRITE(6,20)K,ER,EST,ED
   20 FORMAT(I4,3F12.3)
      WRITE(6,21)A
   21 FORMAT(' A=',E12.5)
      STOP
      END
```

HYP(N,B,C,X) is used to evaluate the hypergeometric function $_2F_1$ (N,B,C,X), where N is a negative integer. The hypergeometric function is in turn used to calculate the Franck-Condon overlap integral, as described in Appendix II. The computational method takes advantage of the proportionality of the hypergeometric function whose first argument is a negative integer to a Jacobi polynomial. The Jacobi polynomial may then be evaluated by standard techniques (56).

```
      DOUBLE PRECISION FUNCTION HYP(N,B,C,X)
      DOUBLE PRECISION X,B,C,Z,AN,ALFA,BETA,AA,BB,CC
      NA=-1*N
      AN=NA*1.0D0
      ALFA=C-1.0D0
      BETA=-1*(AN+B)
      Z=(1.0D0+X)/(1.0D0-X)
      AA=1.0D0
      IF(N)100,999,100
  100 NN=NA-1
      DO 200 L=0,NN
      M=NA-L
      BB=(NA-M+1)*(ALFA+BETA+((NA+M)*1.0D0))
      CC=2*M*(ALFA+(M*1.0D0))
      AA=1.0D0-((BB/CC)*(1.0D0-Z)*AA)
  200 CONTINUE
  999 HYP=AA*(((1.0D0+Z)/2)**N)
      RETURN
      END
```

APPENDIX II

MATHEMATICAL DETAILS

This appendix will present in somewhat greater detail the mathematical formalisms which were used earlier in this work but which, for the sake of clarity and continuity, were not explained in detail.

The general eigenfunctions of the two-dimensional harmonic oscillator are presented. These eigenfunctions are then generalized to approximate the bending eigenfunctions of a nonlinear triatomic molecule by including a term of the form $\frac{a^2}{x^2}$ in the bending potential function. The eigenfunctions thus obtained may be used to represent the ground state, and to calculate Franck-Condon overlap integrals between the two states.

Finally, an approximate treatment is presented of the Renner effect on a triatomic molecule with non-linear geometry. This treatment describes quantitatively the basis for the correlation diagram and quenching curves given in Chapter IV.

The time-independent Schroedinger equation for the isotropic two-dimensional harmonic oscillator may be written in polar co-ordinates:

$$\frac{1}{x}\frac{\partial}{\partial x}\left(x\frac{\partial\Psi}{\partial x}\right)+\frac{1}{x^2}\;\frac{\partial^2\Psi}{\partial\varphi^2}+\frac{8\pi^2 m}{h^2}\;(E-2\pi^2 m\nu^2 x^2)\Psi = 0$$

Here x is the radial co-ordinate, or the component of the S-O distance normal to the figure axis in this application, expressed in centimeters;

φ is the angular co-ordinate, or the angle that the plane of the O-S-O bend makes with some arbitrary but fixed plane; m is the reduced mass of the system in grams; ν is the classical oscillator frequency in Hertz, equal to $\frac{1}{2\pi}\sqrt{\frac{k}{m}}$; h is Planck's constant in erg-sec; and E is the energy of the system in ergs.

Letting $r = 2\pi\sqrt{m\nu/h}\, x$ and $\Psi = R(r)\Phi(\varphi)$, we arrive at the pair of equations

$$\frac{d^2\Phi}{d\varphi^2} = -\ell^2\Phi \quad \text{and}$$

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \left(\lambda - r^2 - \frac{\ell^2}{r^2}\right) R = 0, \text{ where } \lambda = \frac{2E}{h\nu} .$$

The former has single-valued solutions only when ℓ is integral; this is the origin of the quantization of vibrational angular momentum about the figure axis. The solutions of the latter may be expressed conveniently in terms of the variable $\rho = r^2$.

The well-behaved solutions of the radial equation are then

$$R(\rho) = N_{n,\ell}\, \rho^{\frac{|\ell|}{2}} e^{-\frac{\rho}{2}} L^{(|\ell|)}_{\frac{\lambda}{4} - \frac{|\ell|+1}{2}}(\rho)$$

where $\frac{\lambda}{4} - \frac{|\ell|+1}{2}$ must be a non-negative integer, which we shall call n. $L_n^{(a)}(\rho)$ is called the generalized Laguerre polynomial (or simply the Laguerre polynomial) and is not to be confused with the associated Laguerre polynomial which, unfortunately, is given the same conventional notation (herein denoted by $\mathcal{L}_n^{(a)}(x)$). The two are related by the formula

$$L_n^{(a)}(x) \propto \mathcal{L}_{n+a}^{(a)}(x)$$

The energy of the oscillator is quantized by the requirement that n be an integer:

$$\frac{\lambda}{4} - \frac{|\ell|+1}{2} = n$$

$$\lambda - 2|\ell| - 2 = 4n$$

$$\lambda = \frac{2E}{h\nu} = 4n+2+2|\ell|$$

$$E = h\nu\,(2n+1+|\ell|)$$

and n is therefore related to the conventional linear molecule vibrational quantum number, v_2, by the equation

$$v_2 = 2n+|\ell|, \text{ or}$$

$$n = \frac{v_2-|\ell|}{2}$$

The normalization constant for the radial wave function, $N_{n,\ell}$, is given by

$$N_{n,\ell} = \left(\frac{n!}{(n+|\ell|)!}\right)^{\frac{1}{2}} .$$

The expectation value of ρ (or x^2) must be determined by evaluating the integral

$$N^2_{n,\ell} \int_0^{\infty} e^{-\rho} \rho^{|\ell|+1} L_n^{(|\ell|)}(\rho) L_n^{(|\ell|)}(\rho) d\rho$$

According to Buchholz (55), this integral is evaluated as

$$N^2_{n,\ell} \frac{(-1)^n (n+|\ell|)!}{n!} \sum_{j=0}^{n} \binom{1}{n-1} \frac{(|\ell|+j+1)!}{(|\ell|+j)!} \cdot P_j^{(|\ell|,1)}(-1)$$

$$= N^2_{n,\ell}(-1)^n \frac{(n+|\ell|)!}{n!} \left[(n+|\ell|) P_{n-1}^{(|\ell|,1)}(-1) + (n+|\ell|+1) P_n^{(|\ell|,1)}(-1) \right]$$

$$= (-1)^n \left[(n+|\ell|)(-1)^{n-1}(n) + (n+|\ell|+1)(-1)^n (n+1) \right]$$

$$= (n+|\ell|+1)(n+1) - (n+|\ell|)\ (n)$$

$$= \left[\left(\frac{v_2}{2}+1\right)^2 - \ell^2 \right] - \left[\left(\frac{v_2}{2}\right)^2 - \ell^2 \right]$$

$$= v_2+1$$

We wish to calculate Franck-Condon overlap integrals for the transition of a triatomic molecule from a bent to a linear electronic state. Since we wish to consider cold absorption, we need consider only transitions from the lowest vibrational state of the bent molecule. We will represent the potential functions for the bending vibrations of both the ground state and the excited state as isotropic functions of a rectilinear displacement normal to the figure axis. (Hougen, Bunker, and Johns have shown that it is physically more meaningful to consider a Hamiltonian in terms of a curvilinear bending co-ordinate, but we feel that, in the case of sulfur dioxide, the assumption of a harmonic potential for the excited state limits the accuracy of the calculation more than the assumption of rectilinear co-ordinates.)

The excited state potential function will be represented as a simple two-dimensional isotropic harmonic oscillator

$$V(x) = + \tfrac{1}{2}kx^2$$

while the ground state potential function will be represented as a harmonic oscillator perturbed by a term in $1/x^2$:

$$V(x) = + \tfrac{1}{2}fx^2 + \frac{a^2}{x^2}$$

This potential function is admittedly less physically realistic than one with a finite hump in the linear molecular geometry, such as those used by Dixon or Johns. The barrier to linearity is known to be quite large in SO_2, however, and it is unreasonable to believe that tunneling will occur to a significant enough extent to affect the wavefunctions of the ground vibrational state noticeably.

The potential function we have chosen for the ground state has, moreover, the advantage that exact solutions to the Schroedinger equation can be obtained. The method of solution is entirely analogous to that of the two-dimensional harmonic oscillator, and will involve the quantities

$$\nu_f = \frac{1}{2\pi} \left(\frac{f}{n}\right)^{\frac{1}{2}}$$

$$Q^2 = \frac{8\pi^2 a^2 m}{h^2}$$

$$\sigma = \frac{4\pi^2 m \nu_f}{h} x^2$$

$$\lambda = \frac{2E}{h\nu_f}$$

$$\kappa = (K^2 + Q^2)^{\frac{1}{2}}$$

$$M_{n,K} = \left(\frac{n!}{\Gamma(n+\kappa+1)}\right)^{\frac{1}{2}}$$

The solutions of the radial part of the Schroedinger equation will be

$$R(\sigma) = M_{n,K}\, e^{-\frac{\sigma}{2}}\, \sigma^{\frac{\kappa}{2}}\, L^{(\kappa)}_{\frac{\lambda}{4}-\frac{\kappa+1}{2}}(\rho)$$

and they will have energy given by

$$E = h\nu_f\,(2n+\kappa+1)$$

ν_f is related to the equilibrium vibrational frequency of the bent molecule by

$$2\nu_f = \nu_e$$

and n is equal to the conventional vibrational quantum number for the bent molecule, v_2^b.

The general Franck-Condon overlap integral will be

$$I = \int_0^\infty N_{n'\ell'} M_{n''K''} e^{-\frac{\rho+\sigma}{2}} \rho^{\frac{|\ell'|}{2}} \sigma^{\frac{\kappa}{2}} L_{n'}^{(|\ell'|)}(\rho) L_{n''}^{(\kappa)}(\sigma)\, d\rho$$

This integral will in general be quite difficult to evaluate, but the problem is simplified considerably by considering transitions from only the ground vibrational state, since $L_0^{(a)}(x)=1$ for all values of a and x. Setting $b\rho = \sigma$ where $b = \nu_f''/\nu' = \nu_e''/2\nu'$, the desired integral becomes

$$I = N_{n,\ell'} M_{0,K''} \int_0^\infty e^{-\frac{(1+b)}{2}\rho} b^{\frac{\kappa}{2}} \rho^{\frac{|\ell|+\kappa}{2}} L_n^{(|\ell'|)}(\rho)\, d\rho$$

$$= N_{n,\ell'} M_{0,K''} \frac{\Gamma(\frac{|\ell|+\kappa}{2}+n+1)}{n!} \frac{(\frac{b-1}{2})^n}{(\frac{b+1}{2})^{n+1+\frac{|\ell|+\kappa}{2}}} \left\{ {}_2F_1\left[-n, -\frac{\kappa-|\ell|}{2}; -\frac{\kappa+|\ell|}{2}-n; (\frac{b+1}{b-1})\right]\right\}$$

The hypergeometric function, ${}_2F_1$, whose first argument is a negative integer, is proportional to a Jacobi polynomial, and may be evaluated by the methods described by Abramowitz (56). The gamma function may be approximated well using Stirling's approximation. Details of the computer program used to evaluate these integrals may be found in Appendix I.

The rearrangement of rotational levels of a bent molecule due to Renner-Teller coupling may be approximated by applying a perturbing Hamiltonian of the form

$$H' = \eta \rho^2 \left(e^{4i\alpha} + e^{-4i\alpha}\right)$$

(recalling that $\rho^2 \propto x^4$) to the eigenfunctions of the isotropic two-dimensional oscillator with a potential maximum at $\rho = 0$. The non-vanishing matrix elements of this perturbing Hamiltonian will be

$$\langle 2 | \langle n, k-2 | H' | n', k+2 \rangle | -2 \rangle$$

$$= \eta \int_0 R_{n,k-2}(\rho)\, \rho^2\, R_{n',k+2}(\rho)\, d\rho$$

$$\langle -2 | \langle n, k+2 | H' | n', k-2 \rangle | 2 \rangle$$

$$= \eta \int_0 R_{n,k+2}(\rho)\, \rho^2\, R_{n',k-2}(\rho)\, d\rho$$

Although these integrals are, in general, quite difficult to evaluate, a qualitative idea of the kind of rearrangement that takes place may be obtained by making the following approximations:

(1) Ignore all matrix elements involving different values of v_2^b. This approximation assumes that rotational spacings and Renner-Teller coupling both are small compared with vibrational spacing. This approximation limits the accuracy with which the term values of the two electronic components can simultaneously be approximated: the zeroth-order potential function can, of course, be chosen so as to approximate the potential function of either the upper or lower component. Dixon (37) has demonstrated that changes in the equilibrium position or barrier height (such as would be necessary to approximate the potential function of the other component) involve a mixing of basis functions with different values of v_2^b.

(2) Ignore centrifugal distortion. This is equivalent to saying that the radial function $R_{n,\ell}(\rho)$ is not a function of ℓ. In the oscillator defined above by $V(x) = \frac{1}{2}kx^2 + \frac{a^2}{x^2}$, this implies $\kappa = (Q^2+\ell^2)^{\frac{1}{2}}$ is approximately constant. The matrix elements $\eta\int_0^\infty R_{n,k-2}(\rho)\rho^2 R_{n,k+2}(\rho)\,d\rho$ will then be approximated as a constant, which we shall denote γ.

Denoting the eigenvalues of the unperturbed Hamiltonian by $W(k-\Lambda)$, the Hamiltonian matrix becomes a series of 2x2 diagonal blocks of the form

$$\begin{pmatrix} W(k+2) & \gamma \\ \gamma & W(k-2) \end{pmatrix}$$

These matrices may be diagonalized easily to give the qualitative correlation diagram of Figure 9. Notice that, for large γ, the energy approaches $\pm\gamma + AK^2 + 4$ as an asymptote.

It is also useful to plot the expectation value of electronic orbital angular momentum as a function of γ/A. The electronic orbital angular momentum will be "quenched" as γ increases, since eigenvectors of the Hamiltonian matrix will approach the limiting form $2^{-\frac{1}{2}}(\langle 2| \langle v_2^b, k-2| \pm \langle -2| \langle v_2^b, k+2|)$. This quenching will be a function of γ/A and K, as illustrated in Figure 10 .

APPENDIX III

OBSERVED AND CALCULATED ROTATIONAL STRUCTURE

The following appendix tabulates the assigned and calculated rotational structure for the ^pP and ^rR branches of the bands of sulfur dioxide that have been analyzed. The tabulation was generated by the computer programs FIT and ODDFIT described in Appendix I.

For each analyzed band, the following information is given: the band name, the band origin, the calculated rotational constants B' and A'-C', the number of lines assigned, and the accuracy with which these assigned lines could be reproduced by a symmetric rotor energy formula. This information is followed by a list of observed and calculated frequencies for all assigned lines. Finally, the calculated positions of all ^pP and ^rR lines with $0 \leq K < 20$ and $K \leq J \leq K+10$ are presented and, where appropriate, compared with the observed line position. An entry of ".00" in this part of the table means that the transition was not assigned.

The bands analyzed were the B, C, E, F, and G bands of SO_2^{16} and the A, B, E, F, and G bands of SO_2^{18}.

Table 5. Observed and Calculated Transition Frequencies in cm^{-1} for the B Band of SO_2^{16}.

BAND ORIGIN AT 32178.468 CM-1.

B= .319765

A-C= 1.474936

DK= .000000000000

DJK= .000000000000

DJ= .000000000000

ROOT MEAN SQUARE DEVIATION= .1254 CM-1 FOR 34 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	14	14	15	15	32077.800	32077.898	-.098
2	15	14	16	15	32077.200	32077.258	-.058
3	16	14	17	15	32076.600	32076.617	-.017
4	17	14	18	15	32076.000	32075.977	.023
5	18	14	19	15	32075.300	32075.336	-.036
6	12	12	13	13	32096.250	32096.303	-.053
7	13	12	14	13	32095.600	32095.668	-.068
8	14	12	15	13	32095.000	32095.033	-.033
9	16	12	17	13	32094.100	32093.763	.337
10	17	12	18	13	32093.000	32093.129	-.129
11	10	10	11	11	32113.500	32113.511	-.011
12	11	10	12	11	32112.800	32112.879	-.079
13	13	10	14	11	32111.600	32111.616	-.016
14	15	10	16	11	32110.600	32110.355	.245
15	8	8	9	9	32129.550	32129.335	.215
16	9	8	10	9	32128.800	32128.705	.095
17	10	8	11	9	32128.100	32128.075	.025
18	11	8	12	9	32127.500	32127.445	.055
19	12	8	13	9	32126.950	32126.815	.135
20	7	6	8	7	32143.110	32142.988	.123
21	8	6	9	7	32142.200	32142.357	-.157
22	9	6	10	7	32141.700	32141.727	-.027
23	10	6	11	7	32141.000	32141.098	-.098
24	11	6	12	7	32140.400	32140.468	-.068
25	12	6	13	7	32139.700	32139.838	-.138
26	4	4	5	5	32156.050	32156.235	-.185
27	5	4	6	5	32155.500	32155.602	-.102
28	8	4	9	5	32153.600	32153.708	-.107
29	9	4	10	5	32153.000	32153.075	-.075
30	10	4	11	5	32152.300	32152.443	-.143
31	2	2	1	1	32184.100	32183.966	.134
32	3	2	2	1	32184.600	32184.508	.092
33	4	4	3	3	32189.500	32189.266	.234
34	5	4	4	3	32189.900	32189.910	-.010

Table 5. (Continued).

* * * * * * * * P BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
0	0	1	1	32176.15	.00	.00
1	0	2	1	32175.41	.00	.00
2	0	3	1	32175.00	.00	.00
3	0	4	1	32173.97	.00	.00
4	0	5	1	32173.98	.00	.00
5	0	6	1	32172.45	.00	.00
6	0	7	1	32173.07	.00	.00
7	0	8	1	32170.86	.00	.00
8	0	9	1	32172.31	.00	.00
9	0	10	1	32169.22	.00	.00
10	0	11	1	32171.69	.00	.00
2	2	3	3	32167.09	.00	.00
3	2	4	3	32166.46	.00	.00
4	2	5	3	32165.82	.00	.00
5	2	6	3	32165.19	.00	.00
6	2	7	3	32164.55	.00	.00
7	2	8	3	32163.91	.00	.00
8	2	9	3	32163.28	.00	.00
9	2	10	3	32162.61	.00	.00
10	2	11	3	32161.99	.00	.00
11	2	12	3	32161.27	.00	.00
12	2	13	3	32160.70	.00	.00
4	4	5	5	32156.23	32156.05	-.18
5	4	6	5	32155.60	32155.50	-.10
6	4	7	5	32154.97	.00	.00
7	4	8	5	32154.34	.00	.00
8	4	9	5	32153.71	32153.60	-.11
9	4	10	5	32153.08	32153.00	-.08
10	4	11	5	32152.44	32152.30	-.14
11	4	12	5	32151.81	.00	.00
12	4	13	5	32151.17	.00	.00
13	4	14	5	32150.53	.00	.00
14	4	15	5	32149.89	.00	.00
6	6	7	7	32143.62	.00	.00
7	6	8	7	32142.99	32143.11	.12
8	6	9	7	32142.36	32142.20	-.16
9	6	10	7	32141.73	32141.70	-.03
10	6	11	7	32141.10	32141.00	-.10
11	6	12	7	32140.47	32140.40	-.07
12	6	13	7	32139.84	32139.70	-.14
13	6	14	7	32139.21	.00	.00
14	6	15	7	32138.58	.00	.00
15	6	16	7	32137.95	.00	.00
16	6	17	7	32137.31	.00	.00
8	8	9	9	32129.34	32129.55	.21
9	8	10	9	32128.70	32128.80	.10
10	8	11	9	32128.07	32128.10	.03

Table 5. (Continued).

11	8	12	9	32127.44	32127.50	.06
12	8	13	9	32126.82	32126.95	.13
13	8	14	9	32126.19	.00	.00
14	8	15	9	32125.56	.00	.00
15	8	16	9	32124.93	.00	.00
16	8	17	9	32124.30	.00	.00
17	8	18	9	32123.67	.00	.00
18	8	19	9	32123.04	.00	.00
10	10	11	11	32113.51	32113.50	-.01
11	10	12	11	32112.88	32112.80	-.08
12	10	13	11	32112.25	.00	.00
13	10	14	11	32111.62	32111.60	-.02
14	10	15	11	32110.99	.00	.00
15	10	16	11	32110.35	32110.60	.25
16	10	17	11	32109.72	.00	.00
17	10	18	11	32109.09	.00	.00
18	10	19	11	32108.46	.00	.00
19	10	20	11	32107.83	.00	.00
20	10	21	11	32107.20	.00	.00
12	12	13	13	32096.30	32096.25	-.05
13	12	14	13	32095.67	32095.60	-.07
14	12	15	13	32095.03	32095.00	-.03
15	12	16	13	32094.40	.00	.00
16	12	17	13	32093.76	32094.10	.34
17	12	18	13	32093.13	32093.00	-.13
18	12	19	13	32092.49	.00	.00
19	12	20	13	32091.86	.00	.00
20	12	21	13	32091.23	.00	.00
21	12	22	13	32090.59	.00	.00
22	12	23	13	32089.96	.00	.00
14	14	15	15	32077.90	32077.80	-.10
15	14	16	15	32077.26	32077.20	-.06
16	14	17	15	32076.62	32076.60	-.02
17	14	18	15	32075.98	32076.00	.02
18	14	19	15	32075.34	32075.30	-.04
19	14	20	15	32074.70	.00	.00
20	14	21	15	32074.06	.00	.00
21	14	22	15	32073.41	.00	.00
22	14	23	15	32072.77	.00	.00
23	14	24	15	32072.13	.00	.00
24	14	25	15	32071.49	.00	.00
16	16	17	17	32058.52	.00	.00
17	16	18	17	32057.87	.00	.00
18	16	19	17	32057.22	.00	.00
19	16	20	17	32056.57	.00	.00
20	16	21	17	32055.92	.00	.00
21	16	22	17	32055.27	.00	.00
22	16	23	17	32054.62	.00	.00
23	16	24	17	32053.97	.00	.00
24	16	25	17	32053.32	.00	.00
25	16	26	17	32052.67	.00	.00
26	16	27	17	32052.02	.00	.00

Table 5. (Continued).

18	18	19	19	32038.41	.00	.00
19	18	20	19	32037.75	.00	.00
20	18	21	19	32037.09	.00	.00
21	18	22	19	32036.43	.00	.00
22	18	23	19	32035.77	.00	.00
23	18	24	19	32035.11	.00	.00
24	18	25	19	32034.45	.00	.00
25	18	26	19	32033.79	.00	.00
26	18	27	19	32033.13	.00	.00
27	18	28	19	32032.46	.00	.00
28	18	29	19	32031.80	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
2	2	1	1	32183.97	32184.10	.13
3	2	2	1	32184.51	32184.60	.09
4	2	3	1	32185.38	.00	.00
5	2	4	1	32185.63	.00	.00
6	2	5	1	32186.91	.00	.00
7	2	6	1	32186.66	.00	.00
8	2	7	1	32188.57	.00	.00
9	2	8	1	32187.63	.00	.00
10	2	9	1	32190.36	.00	.00
11	2	10	1	32188.55	.00	.00
12	2	11	1	32192.30	.00	.00
4	4	3	3	32189.27	32189.50	.23
5	4	4	3	32189.91	32189.90	-.01
6	4	5	3	32190.55	.00	.00
7	4	6	3	32191.20	.00	.00
8	4	7	3	32191.84	.00	.00
9	4	8	3	32192.48	.00	.00
10	4	9	3	32193.13	.00	.00
11	4	10	3	32193.74	.00	.00
12	4	11	3	32194.40	.00	.00
13	4	12	3	32194.96	.00	.00
14	4	13	3	32195.67	.00	.00
6	6	5	5	32192.77	.00	.00
7	6	6	5	32193.41	.00	.00
8	6	7	5	32194.06	.00	.00
9	6	8	5	32194.71	.00	.00
10	6	9	5	32195.36	.00	.00
11	6	10	5	32196.00	.00	.00
12	6	11	5	32196.65	.00	.00
13	6	12	5	32197.30	.00	.00
14	6	13	5	32197.94	.00	.00
15	6	14	5	32198.58	.00	.00
16	6	15	5	32199.22	.00	.00
8	8	7	7	32194.51	.00	.00
9	8	8	7	32195.16	.00	.00

Table 5. (Continued).

10	8	9	7	32195.81	.00	.00
11	8	10	7	32196.46	.00	.00
12	8	11	7	32197.10	.00	.00
13	8	12	7	32197.75	.00	.00
14	8	13	7	32198.40	.00	.00
15	8	14	7	32199.05	.00	.00
16	8	15	7	32199.70	.00	.00
17	8	16	7	32200.35	.00	.00
18	8	17	7	32200.99	.00	.00
10	10	9	9	32194.58	.00	.00
11	10	10	9	32195.23	.00	.00
12	10	11	9	32195.88	.00	.00
13	10	12	9	32196.53	.00	.00
14	10	13	9	32197.18	.00	.00
15	10	14	9	32197.83	.00	.00
16	10	15	9	32198.48	.00	.00
17	10	16	9	32199.13	.00	.00
18	10	17	9	32199.78	.00	.00
19	10	18	9	32200.43	.00	.00
20	10	19	9	32201.08	.00	.00
12	12	11	11	32193.12	.00	.00
13	12	12	11	32193.76	.00	.00
14	12	13	11	32194.41	.00	.00
15	12	14	11	32195.06	.00	.00
16	12	15	11	32195.71	.00	.00
17	12	16	11	32196.36	.00	.00
18	12	17	11	32197.00	.00	.00
19	12	18	11	32197.65	.00	.00
20	12	19	11	32198.30	.00	.00
21	12	20	11	32198.95	.00	.00
22	12	21	11	32199.60	.00	.00
14	14	13	13	32190.27	.00	.00
15	14	14	13	32190.91	.00	.00
16	14	15	13	32191.55	.00	.00
17	14	16	13	32192.20	.00	.00
18	14	17	13	32192.84	.00	.00
19	14	18	13	32193.49	.00	.00
20	14	19	13	32194.13	.00	.00
21	14	20	13	32194.78	.00	.00
22	14	21	13	32195.42	.00	.00
23	14	22	13	32196.07	.00	.00
24	14	23	13	32196.71	.00	.00
16	16	15	15	32186.22	.00	.00
17	16	16	15	32186.86	.00	.00
18	16	17	15	32187.50	.00	.00
19	16	18	15	32188.14	.00	.00
20	16	19	15	32188.77	.00	.00
21	16	20	15	32189.41	.00	.00
22	16	21	15	32190.05	.00	.00
23	16	22	15	32190.69	.00	.00
24	16	23	15	32191.33	.00	.00
25	16	24	15	32191.97	.00	.00

Table 5. (Continued).

26	16	25	15	32192.60	.00	.00
18	18	17	17	32181.20	.00	.00
19	18	18	17	32181.83	.00	.00
20	18	19	17	32182.46	.00	.00
21	18	20	17	32183.09	.00	.00
22	18	21	17	32183.72	.00	.00
23	18	22	17	32184.35	.00	.00
24	18	23	17	32184.98	.00	.00
25	18	24	17	32185.61	.00	.00
26	18	25	17	32186.24	.00	.00
27	18	26	17	32186.87	.00	.00
28	18	27	17	32187.49	.00	.00
20	20	19	19	32175.45	.00	.00
21	20	20	19	32176.07	.00	.00
22	20	21	19	32176.69	.00	.00
23	20	22	19	32177.31	.00	.00
24	20	23	19	32177.93	.00	.00
25	20	24	19	32178.54	.00	.00
26	20	25	19	32179.16	.00	.00
27	20	26	19	32179.78	.00	.00
28	20	27	19	32180.40	.00	.00
29	20	28	19	32181.01	.00	.00
30	20	29	19	32181.63	.00	.00

Table 6. Observed and Calculated Transition Frequencies in cm^{-1} for the C Band of SO_2^{16}.

BAND ORIGIN AT 32397.039 CM-1.

B= .311969
A-C= 1.566623
DK= .000000000000
DJK= .000000000000
DJ= .000000000000
ROOT MEAN SQUARE DEVIATION= .1410 CM-1 FOR 45 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	5	5	6	6	32370.600	32370.770	-.170
2	6	5	7	6	32370.000	32370.045	-.045
3	9	5	10	6	32367.500	32367.779	-.279
4	7	7	8	8	32359.210	32359.304	-.094
5	8	7	9	8	32358.600	32358.549	.051
6	9	7	10	8	32357.950	32357.779	.171
7	10	7	11	8	32357.000	32356.993	.007
8	11	7	12	8	32356.100	32356.192	-.092
9	12	7	13	8	32355.500	32355.376	.124
10	9	9	10	10	32347.000	32346.902	.098
11	10	9	11	10	32346.300	32346.115	.185
12	11	9	12	10	32345.470	32345.313	.157
13	12	9	13	10	32344.400	32344.495	-.095
14	13	9	14	10	32344.000	32343.663	.337
15	11	11	12	12	32333.500	32333.704	-.204
16	12	11	13	12	32332.900	32332.884	.016
17	13	11	14	12	32332.100	32332.048	.052
18	14	11	15	12	32331.250	32331.197	.053
19	15	11	16	12	32330.300	32330.331	-.031
20	16	11	17	12	32329.200	32329.449	-.249
21	18	11	19	12	32327.450	32327.639	-.189
22	20	11	21	12	32326.000	32325.766	.234
23	6	5	5	4	32412.500	32412.422	.078
24	8	5	7	4	32413.700	32413.481	.219
25	11	5	10	4	32414.900	32414.946	-.046
26	12	5	11	4	32415.600	32415.400	.200
27	13	5	12	4	32415.600	32415.833	-.233
28	14	5	13	4	32416.200	32416.252	-.052
29	9	7	8	6	32417.400	32417.510	-.111
30	10	7	9	6	32418.200	32418.003	.197
31	14	7	13	6	32419.800	32419.816	-.016
32	16	7	15	6	32420.600	32420.624	-.024
33	17	7	16	6	32421.000	32421.002	-.002
34	9	9	8	8	32419.800	32420.043	-.243
35	10	9	9	8	32420.600	32420.536	.064
36	11	9	10	8	32421.000	32421.013	-.013
37	13	9	12	8	32421.900	32421.923	-.023
38	14	9	13	8	32422.200	32422.354	-.154
39	15	9	14	8	32422.800	32422.770	.030
40	17	9	16	8	32423.600	32423.555	.045
41	19	9	18	8	32424.300	32424.274	.026
42	11	11	10	10	32422.600	32422.670	.130
43	13	11	12	10	32423.600	32423.576	.024
44	15	11	14	10	32424.300	32424.422	-.122
45	17	11	16	10	32425.200	32425.206	-.006

Table 6. (Continued).

* * * * * * * * P BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	2	2	32390.48	.00	.00
2	1	3	2	32389.82	.00	.00
3	1	4	2	32389.12	.00	.00
4	1	5	2	32388.45	.00	.00
5	1	6	2	32387.67	.00	.00
6	1	7	2	32387.04	.00	.00
7	1	8	2	32386.09	.00	.00
8	1	9	2	32385.59	.00	.00
9	1	10	2	32384.33	.00	.00
10	1	11	2	32384.12	.00	.00
11	1	12	2	32382.39	.00	.00
3	3	4	4	32381.19	.00	.00
4	3	5	4	32380.49	.00	.00
5	3	6	4	32379.78	.00	.00
6	3	7	4	32379.06	.00	.00
7	3	8	4	32378.31	.00	.00
8	3	9	4	32377.55	.00	.00
9	3	10	4	32376.78	.00	.00
10	3	11	4	32375.98	.00	.00
11	3	12	4	32375.17	.00	.00
12	3	13	4	32374.34	.00	.00
13	3	14	4	32373.48	.00	.00
5	5	6	6	32370.77	32370.60	-.17
6	5	7	6	32370.04	32370.00	-.04
7	5	8	6	32369.30	.00	.00
8	5	9	6	32368.55	.00	.00
9	5	10	6	32367.78	32367.50	-.28
10	5	11	6	32366.99	.00	.00
11	5	12	6	32366.19	.00	.00
12	5	13	6	32365.37	.00	.00
13	5	14	6	32364.54	.00	.00
14	5	15	6	32363.68	.00	.00
15	5	16	6	32362.81	.00	.00
7	7	8	8	32359.30	32359.21	-.09
8	7	9	8	32358.55	32358.60	.05
9	7	10	8	32357.78	32357.95	.17
10	7	11	8	32356.99	32357.00	.01
11	7	12	8	32356.19	32356.10	-.09
12	7	13	8	32355.38	32355.50	.12
13	7	14	8	32354.54	.00	.00
14	7	15	8	32353.70	.00	.00
15	7	16	8	32352.83	.00	.00
16	7	17	8	32351.95	.00	.00
17	7	18	8	32351.06	.00	.00
9	9	10	10	32346.90	32347.00	.10
10	9	11	10	32346.11	32346.30	.19
11	9	12	10	32345.31	32345.47	.16
12	9	13	10	32344.50	32344.40	-.10
13	9	14	10	32343.66	32344.00	.34
14	9	15	10	32342.81	.00	.00
15	9	16	10	32341.95	.00	.00
16	9	17	10	32341.07	.00	.00

Table 6. (Continued).

17	9	18	10	32340.18	.00	.00
18	9	19	10	32339.27	.00	.00
19	9	20	10	32338.34	.00	.00
11	11	12	12	32333.70	32333.50	-.20
12	11	13	12	32332.88	32332.90	.02
13	11	14	12	32332.05	32332.10	.05
14	11	15	12	32331.20	32331.25	.05
15	11	16	12	32330.33	32330.30	-.03
16	11	17	12	32329.45	32329.20	-.25
17	11	18	12	32328.55	.00	.00
18	11	19	12	32327.64	32327.45	-.19
19	11	20	12	32326.71	.00	.00
20	11	21	12	32325.77	32326.00	.23
21	11	22	12	32324.81	.00	.00
13	13	14	14	32319.88	.00	.00
14	13	15	14	32319.03	.00	.00
15	13	16	14	32318.16	.00	.00
16	13	17	14	32317.27	.00	.00
17	13	18	14	32316.37	.00	.00
18	13	19	14	32315.45	.00	.00
19	13	20	14	32314.52	.00	.00
20	13	21	14	32313.57	.00	.00
21	13	22	14	32312.60	.00	.00
22	13	23	14	32311.62	.00	.00
23	13	24	14	32310.63	.00	.00
15	15	16	16	32305.64	.00	.00
16	15	17	16	32304.75	.00	.00
17	15	18	16	32303.84	.00	.00
18	15	19	16	32302.92	.00	.00
19	15	20	16	32301.98	.00	.00
20	15	21	16	32301.02	.00	.00
21	15	22	16	32300.05	.00	.00
22	15	23	16	32299.06	.00	.00
23	15	24	16	32298.06	.00	.00
24	15	25	16	32297.04	.00	.00
25	15	26	16	32296.00	.00	.00
17	17	18	18	32291.22	.00	.00
18	17	19	18	32290.29	.00	.00
19	17	20	18	32289.34	.00	.00
20	17	21	18	32288.37	.00	.00
21	17	22	18	32287.39	.00	.00
22	17	23	18	32286.39	.00	.00
23	17	24	18	32285.38	.00	.00
24	17	25	18	32284.35	.00	.00
25	17	26	18	32283.30	.00	.00
26	17	27	18	32282.24	.00	.00
27	17	28	18	32281.16	.00	.00
19	19	20	20	32276.88	.00	.00
20	19	21	20	32275.90	.00	.00
21	19	22	20	32274.91	.00	.00
22	19	23	20	32273.90	.00	.00
23	19	24	20	32272.87	.00	.00
24	19	25	20	32271.83	.00	.00
25	19	26	20	32270.77	.00	.00
26	19	27	20	32269.70	.00	.00

Table 6. (Continued).

27	19	28	20	32268.61	.00	.00
28	19	29	20	32267.50	.00	.00
29	19	30	20	32266.38	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	0	0	32399.23	.00	.00
2	1	1	0	32400.48	.00	.00
3	1	2	0	32400.44	.00	.00
4	1	3	0	32404.84	.00	.00
5	1	4	0	32401.60	.00	.00
6	1	5	0	32411.71	.00	.00
7	1	6	0	32402.76	.00	.00
8	1	7	0	32421.07	.00	.00
9	1	8	0	32403.96	.00	.00
10	1	9	0	32432.92	.00	.00
11	1	10	0	32405.24	.00	.00
3	3	2	2	32406.13	.00	.00
4	3	3	2	32406.72	.00	.00
5	3	4	2	32407.27	.00	.00
6	3	5	2	32407.85	.00	.00
7	3	6	2	32408.31	.00	.00
8	3	7	2	32408.93	.00	.00
9	3	8	2	32409.23	.00	.00
10	3	9	2	32409.98	.00	.00
11	3	10	2	32409.97	.00	.00
12	3	11	2	32411.00	.00	.00
13	3	12	2	32410.52	.00	.00
5	5	4	4	32411.87	.00	.00
6	5	5	4	32412.42	32412.50	.08
7	5	6	4	32412.96	.00	.00
8	5	7	4	32413.48	32413.70	.22
9	5	8	4	32413.99	.00	.00
10	5	9	4	32414.47	.00	.00
11	5	10	4	32414.95	32414.90	-.05
12	5	11	4	32415.40	32415.60	.20
13	5	12	4	32415.83	32415.60	-.23
14	5	13	4	32416.25	32416.20	-.05
15	5	14	4	32416.64	.00	.00
7	7	6	6	32416.48	.00	.00
8	7	7	6	32417.00	.00	.00
9	7	8	6	32417.51	32417.40	-.11
10	7	9	6	32418.00	32418.20	.20
11	7	10	6	32418.48	.00	.00
12	7	11	6	32418.94	.00	.00
13	7	12	6	32419.39	.00	.00
14	7	13	6	32419.82	32419.80	-.02
15	7	14	6	32420.23	.00	.00
16	7	15	6	32420.62	32420.60	-.02
17	7	16	6	32421.00	32421.00	-.00
9	9	8	8	32420.04	32419.80	-.24
10	9	9	8	32420.54	32420.60	.06
11	9	10	8	32421.01	32421.00	-.01
12	9	11	8	32421.48	.00	.00
13	9	12	8	32421.92	32421.90	-.02

Table 6. (Continued).

14	9	13	8	32422.35	32422.20	-.15
15	9	14	8	32422.77	32422.80	.03
16	9	15	8	32423.17	.00	.00
17	9	16	8	32423.55	32423.60	.05
18	9	17	8	32423.92	.00	.00
19	9	18	8	32424.27	32424.30	.03
11	11	10	10	32422.67	32422.80	.13
12	11	11	10	32423.13	.00	.00
13	11	12	10	32423.58	32423.60	.02
14	11	13	10	32424.01	.00	.00
15	11	14	10	32424.42	32424.30	-.12
16	11	15	10	32424.82	.00	.00
17	11	16	10	32425.21	32425.20	-.01
18	11	17	10	32425.57	.00	.00
19	11	18	10	32425.93	.00	.00
20	11	19	10	32426.27	.00	.00
21	11	20	10	32426.59	.00	.00
13	13	12	12	32424.50	.00	.00
14	13	13	12	32424.93	.00	.00
15	13	14	12	32425.34	.00	.00
16	13	15	12	32425.74	.00	.00
17	13	16	12	32426.12	.00	.00
18	13	17	12	32426.48	.00	.00
19	13	18	12	32426.84	.00	.00
20	13	19	12	32427.17	.00	.00
21	13	20	12	32427.49	.00	.00
22	13	21	12	32427.79	.00	.00
23	13	22	12	32428.08	.00	.00
15	15	14	14	32425.71	.00	.00
16	15	15	14	32426.10	.00	.00
17	15	16	14	32426.48	.00	.00
18	15	17	14	32426.84	.00	.00
19	15	18	14	32427.18	.00	.00
20	15	19	14	32427.51	.00	.00
21	15	20	14	32427.83	.00	.00
22	15	21	14	32428.13	.00	.00
23	15	22	14	32428.41	.00	.00
24	15	23	14	32428.68	.00	.00
25	15	24	14	32428.93	.00	.00
17	17	16	16	32426.50	.00	.00
18	17	17	16	32426.85	.00	.00
19	17	18	16	32427.19	.00	.00
20	17	19	16	32427.51	.00	.00
21	17	20	16	32427.82	.00	.00
22	17	21	16	32428.11	.00	.00
23	17	22	16	32428.39	.00	.00
24	17	23	16	32428.65	.00	.00
25	17	24	16	32428.89	.00	.00
26	17	25	16	32429.12	.00	.00
27	17	26	16	32429.33	.00	.00
19	19	18	18	32427.10	.00	.00
20	19	19	18	32427.42	.00	.00
21	19	20	18	32427.71	.00	.00
22	19	21	18	32428.00	.00	.00
23	19	22	18	32428.26	.00	.00

Table 6. (Continued).

24	19	23	18	32428.51	.00	.00
25	19	24	18	32428.75	.00	.00
26	19	25	18	32428.97	.00	.00
27	19	26	18	32429.17	.00	.00
28	19	27	18	32429.35	.00	.00
29	19	28	18	32429.53	.00	.00

Table 7. Observed and Calculated Transition Frequencies in cm^{-1} for the E Band of SO_2^{16}.

BAND ORIGIN AT 32865.890 CM-1.
B= .322528
A-C= 1.511880
DK= .000000000000
DJK= .000000000000
DJ= .000000000000
ROOT MEAN SQUARE DEVIATION= .1199 CM-1 FOR 46 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	3	3	4	4	32849.700	32849.674	.026
2	4	3	5	4	32849.200	32849.062	.138
3	5	3	6	4	32848.590	32848.458	.132
4	6	3	7	4	32847.780	32847.858	-.078
5	7	3	8	4	32847.030	32847.263	-.233
6	8	3	9	4	32846.600	32846.673	-.073
7	9	3	10	4	32846.210	32846.086	.124
8	5	5	6	6	32838.550	32838.569	-.020
9	6	5	7	6	32837.890	32837.971	-.081
10	8	5	9	6	32836.670	32836.792	-.123
11	9	5	10	6	32836.100	32836.212	-.112
12	8	7	9	8	32825.400	32825.478	-.078
13	10	7	11	8	32824.400	32824.323	.077
14	11	11	12	12	32797.500	32797.325	.175
15	12	11	13	12	32796.660	32796.758	-.098
16	13	11	14	12	32796.190	32796.197	-.007
17	14	11	15	12	32795.710	32795.642	.068
18	13	13	14	14	32781.310	32781.405	-.095
19	14	13	15	14	32780.800	32780.845	-.045
20	15	13	16	14	32780.290	32780.290	.000
21	16	13	17	14	32779.890	32779.741	.149
22	17	13	18	14	32779.180	32779.198	-.018
23	3	3	2	2	32874.810	32874.620	.190
24	4	3	3	2	32875.400	32875.288	.112
25	5	3	4	2	32875.910	32875.947	-.037
26	6	3	5	2	32876.600	32876.648	-.048
27	7	3	6	2	32877.000	32877.264	-.264
28	8	3	7	2	32877.990	32878.047	-.057
29	9	3	8	2	32878.700	32878.536	.165
30	10	3	9	2	32879.500	32879.497	.003
31	5	5	4	4	32879.700	32879.669	.031
32	6	5	5	4	32880.350	32880.349	.001
33	8	5	7	4	32881.720	32881.724	-.003
34	10	5	9	4	32883.150	32883.119	.031
35	7	7	6	6	32883.620	32883.240	.380
36	8	7	7	6	32883.900	32883.932	-.032
37	9	7	8	6	32884.480	32884.630	-.150
38	10	7	9	6	32885.400	32885.333	.066
39	11	7	10	6	32886.000	32886.043	-.043
40	13	7	12	6	32887.490	32887.478	.012
41	11	11	10	10	32886.260	32886.291	-.031
42	13	11	12	10	32887.500	32887.726	-.226
43	14	11	13	10	32888.510	32888.452	.058
44	13	13	12	12	32885.900	32886.022	-.122
45	15	13	14	12	32887.480	32887.474	.006
46	16	13	15	12	32888.350	32888.209	.141

Table 7. (Continued).

* * * * * * * * P BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	2	2	32859.30	.00	.00
2	1	3	2	32858.68	.00	.00
3	1	4	2	32858.05	.00	.00
4	1	5	2	32857.46	.00	.00
5	1	6	2	32856.78	.00	.00
6	1	7	2	32856.28	.00	.00
7	1	8	2	32855.47	.00	.00
8	1	9	2	3285[illegible].15	.00	.00
9	1	10	2	32854.08	.00	.00
10	1	11	2	32854.08	.00	.00
11	1	12	2	32852.58	.00	.00
3	3	4	4	32849.67	32849.70	.03
4	3	5	4	32849.06	32849.20	.14
5	3	6	4	32848.46	32848.59	.13
6	3	7	4	32847.86	32847.78	-.08
7	3	8	4	32847.26	32847.03	-.23
8	3	9	4	32846.67	32846.60	-.07
9	3	10	4	32846.09	32846.21	.12
10	3	11	4	32845.50	.00	.00
11	3	12	4	32844.92	.00	.00
12	3	13	4	32844.35	.00	.00
13	3	14	4	32843.76	.00	.00
5	5	6	6	32838.57	32838.55	-.02
6	5	7	6	32837.97	32837.89	-.08
7	5	8	6	32837.38	.00	.00
8	5	9	6	32836.79	32836.67	-.12
9	5	10	6	32836.21	32836.10	-.11
10	5	11	6	32835.64	.00	.00
11	5	12	6	32835.07	.00	.00
12	5	13	6	32834.50	.00	.00
13	5	14	6	32833.94	.00	.00
14	5	15	6	32833.38	.00	.00
15	5	16	6	32832.83	.00	.00
7	7	8	8	32826.06	.00	.00
8	7	9	8	32825.48	32825.40	-.08
9	7	10	8	32824.90	.00	.00
10	7	11	8	32824.32	32824.40	.08
11	7	12	8	32823.75	.00	.00
12	7	13	8	32823.19	.00	.00
13	7	14	8	32822.63	.00	.00
14	7	15	8	32822.08	.00	.00
15	7	16	8	32821.54	.00	.00
16	7	17	8	32820.99	.00	.00
17	7	18	8	32820.46	.00	.00
9	9	10	10	32812.27	.00	.00
10	9	11	10	32811.69	.00	.00
11	9	12	10	32811.12	.00	.00
12	9	13	10	32810.56	.00	.00
13	9	14	10	32810.00	.00	.00
14	9	15	10	32809.45	.00	.00

Table 7. (Continued).

15	9	16	10	32808.90	.00	.00
16	9	17	10	32808.36	.00	.00
17	9	18	10	32807.83	.00	.00
18	9	19	10	32807.29	.00	.00
19	9	20	10	32806.77	.00	.00
11	11	12	12	32797.33	32797.50	.17
12	11	13	12	32796.76	32796.66	-.10
13	11	14	12	32796.20	32796.19	-.01
14	11	15	12	32795.64	32795.71	.07
15	11	16	12	32795.09	.00	.00
16	11	17	12	32794.55	.00	.00
17	11	18	12	32794.01	.00	.00
18	11	19	12	32793.48	.00	.00
19	11	20	12	32792.95	.00	.00
20	11	21	12	32792.43	.00	.00
21	11	22	12	32791.91	.00	.00
13	13	14	14	32781.40	32781.31	-.09
14	13	15	14	32780.84	32780.80	-.04
15	13	16	14	32780.29	32780.29	.00
16	13	17	14	32779.74	32779.89	.15
17	13	18	14	32779.20	32779.18	-.02
18	13	19	14	32778.66	.00	.00
19	13	20	14	32778.13	.00	.00
20	13	21	14	32777.60	.00	.00
21	13	22	14	32777.08	.00	.00
22	13	23	14	32776.56	.00	.00
23	13	24	14	32776.05	.00	.00
15	15	16	16	32764.71	.00	.00
16	15	17	16	32764.16	.00	.00
17	15	18	16	32763.61	.00	.00
18	15	19	16	32763.06	.00	.00
19	15	20	16	32762.52	.00	.00
20	15	21	16	32761.99	.00	.00
21	15	22	16	32761.46	.00	.00
22	15	23	16	32760.94	.00	.00
23	15	24	16	32760.42	.00	.00
24	15	25	16	32759.91	.00	.00
25	15	26	16	32759.40	.00	.00
17	17	18	18	32747.48	.00	.00
18	17	19	18	32746.93	.00	.00
19	17	20	18	32746.38	.00	.00
20	17	21	18	32745.84	.00	.00
21	17	22	18	32745.30	.00	.00
22	17	23	18	32744.76	.00	.00
23	17	24	18	32744.24	.00	.00
24	17	25	18	32743.71	.00	.00
25	17	26	18	32743.20	.00	.00
26	17	27	18	32742.68	.00	.00
27	17	28	18	32742.18	.00	.00
19	19	20	20	32729.98	.00	.00
20	19	21	20	32729.42	.00	.00
21	19	22	20	32728.88	.00	.00

Table 7. (Continued).

22	19	23	20	32728.33	.00	.00
23	19	24	20	32727.79	.00	.00
24	19	25	20	32727.26	.00	.00
25	19	26	20	32726.73	.00	.00
26	19	27	20	32726.20	.00	.00
27	19	28	20	32725.68	.00	.00
28	19	29	20	32725.16	.00	.00
29	19	30	20	32724.65	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	0	0	32868.05	.00	.00
2	1	1	0	32869.34	.00	.00
3	1	2	0	32869.36	.00	.00
4	1	3	0	32873.85	.00	.00
5	1	4	0	32870.72	.00	.00
6	1	5	0	32880.95	.00	.00
7	1	6	0	32872.15	.00	.00
8	1	7	0	32890.62	.00	.00
9	1	8	0	32873.70	.00	.00
10	1	9	0	32902.88	.00	.00
11	1	10	0	32875.43	.00	.00
3	3	2	2	32874.62	32874.81	.19
4	3	3	2	32875.29	32875.40	.11
5	3	4	2	32875.95	32875.91	-.04
6	3	5	2	32876.65	32876.60	-.05
7	3	6	2	32877.26	32877.00	-.26
8	3	7	2	32878.05	32877.99	-.06
9	3	8	2	32878.54	32878.70	.16
10	3	9	2	32879.50	32879.50	.00
11	3	10	2	32879.72	.00	.00
12	3	11	2	32881.01	.00	.00
13	3	12	2	32880.80	.00	.00
5	5	4	4	32879.67	32879.70	.03
6	5	5	4	32880.35	32880.35	.00
7	5	6	4	32881.03	.00	.00
8	5	7	4	32881.72	32881.72	-.00
9	5	8	4	32882.42	.00	.00
10	5	9	4	32883.12	32883.15	.03
11	5	10	4	32883.82	.00	.00
12	5	11	4	32884.53	.00	.00
13	5	12	4	32885.24	.00	.00
14	5	13	4	32885.95	.00	.00
15	5	14	4	32886.66	.00	.00
7	7	6	6	32883.24	32883.62	.38
8	7	7	6	32883.93	32883.90	-.03
9	7	8	6	32884.63	32884.48	-.15
10	7	9	6	32885.33	32885.40	.07
11	7	10	6	32886.04	32886.00	-.04
12	7	11	6	32886.76	.00	.00
13	7	12	6	32887.48	32887.49	.01
14	7	13	6	32888.20	.00	.00
15	7	14	6	32888.93	.00	.00
16	7	15	6	32889.67	.00	.00

Table 7. (Continued).

17	7	16	6	32890.40	.00	.00
9	9	8	8	32885.41	.00	.00
10	9	9	8	32886.11	.00	.00
11	9	10	8	32886.82	.00	.00
12	9	11	8	32887.54	.00	.00
13	9	12	8	32888.26	.00	.00
14	9	13	8	32888.99	.00	.00
15	9	14	8	32889.72	.00	.00
16	9	15	8	32890.46	.00	.00
17	9	16	8	32891.20	.00	.00
18	9	17	8	32891.95	.00	.00
19	9	18	8	32892.70	.00	.00
11	11	10	10	32886.29	32886.26	-.03
12	11	11	10	32887.01	.00	.00
13	11	12	10	32887.73	32887.50	-.23
14	11	13	10	32888.45	32888.51	.06
15	11	14	10	32889.18	.00	.00
16	11	15	10	32889.92	.00	.00
17	11	16	10	32890.66	.00	.00
18	11	17	10	32891.41	.00	.00
19	11	18	10	32892.17	.00	.00
20	11	19	10	32892.93	.00	.00
21	11	20	10	32893.69	.00	.00
13	13	12	12	32886.02	32885.90	-.12
14	13	13	12	32886.75	.00	.00
15	13	14	12	32887.47	32887.48	.01
16	13	15	12	32888.21	32888.35	.14
17	13	16	12	32888.95	.00	.00
18	13	17	12	32889.70	.00	.00
19	13	18	12	32890.45	.00	.00
20	13	19	12	32891.20	.00	.00
21	13	20	12	32891.97	.00	.00
22	13	21	12	32892.74	.00	.00
23	13	22	12	32893.51	.00	.00
15	15	14	14	32884.78	.00	.00
16	15	15	14	32885.51	.00	.00
17	15	16	14	32886.24	.00	.00
18	15	17	14	32886.98	.00	.00
19	15	18	14	32887.73	.00	.00
20	15	19	14	32888.48	.00	.00
21	15	20	14	32889.24	.00	.00
22	15	21	14	32890.00	.00	.00
23	15	22	14	32890.77	.00	.00
24	15	23	14	32891.55	.00	.00
25	15	24	14	32892.33	.00	.00
17	17	16	16	32882.76	.00	.00
18	17	17	16	32883.49	.00	.00
19	17	18	16	32884.23	.00	.00
20	17	19	16	32884.98	.00	.00
21	17	20	16	32885.73	.00	.00
22	17	21	16	32886.49	.00	.00
23	17	22	16	32887.25	.00	.00

Table 7. (Continued).

24	17	23	16	32888.01	.00	.00
25	17	24	16	32888.79	.00	.00
26	17	25	16	32889.56	.00	.00
27	17	26	16	32890.35	.00	.00
19	19	18	18	32880.20	.00	.00
20	19	19	18	32880.94	.00	.00
21	19	20	18	32881.68	.00	.00
22	19	21	18	32882.43	.00	.00
23	19	22	18	32883.18	.00	.00
24	19	23	18	32883.94	.00	.00
25	19	24	18	32884.70	.00	.00
26	19	25	18	32885.47	.00	.00
27	19	26	18	32886.24	.00	.00
28	19	27	18	32887.02	.00	.00
29	19	28	18	32887.80	.00	.00

Table 8. Observed and Calculated Transition Frequencies in cm^{-1} for the F Band of SO_2^{16}.

BAND ORIGIN AT 33098.385 CM-1.
B= .321231
A-C= 1.500143
DK= .000000000000
DJK= .000000000000
DJ= .000000000000
ROOT MEAN SQUARE DEVIATION= .1269 CM-1 FOR 45 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	4	4	5	5	33076.570	33076.583	-.013
2	6	6	7	7	33064.870	33064.503	.367
3	8	6	9	7	33063.200	33063.286	-.086
4	8	8	9	9	33050.650	33050.970	-.320
5	9	8	10	9	33050.100	33050.366	-.266
6	10	8	11	9	33049.600	33049.765	-.165
7	10	10	11	11	33036.280	33036.109	.170
8	11	10	12	11	33035.780	33035.509	.271
9	12	10	13	11	33034.990	33034.913	.077
10	13	10	14	11	33034.370	33034.320	.050
11	12	12	13	13	33020.030	33020.077	-.047
12	13	12	14	13	33019.300	33019.480	-.180
13	14	12	15	13	33018.900	33018.886	.014
14	16	12	17	13	33017.720	33017.708	.012
15	17	12	18	13	33017.150	33017.123	.027
16	18	12	19	13	33016.580	33016.542	.039
17	20	12	21	13	33015.300	33015.387	-.087
18	14	14	15	15	33002.990	33003.062	-.072
19	15	14	16	15	33002.500	33002.466	.034
20	16	14	17	15	33001.990	33001.873	.118
21	17	14	18	15	33001.290	33001.282	.008
22	18	14	19	15	33000.680	33000.694	-.014
23	4	4	3	3	33109.400	33109.614	-.214
24	5	4	4	3	33110.300	33110.273	.026
25	6	4	5	3	33110.900	33110.936	-.036
26	7	4	6	3	33111.600	33111.600	.000
27	8	4	7	3	33112.400	33112.268	.132
28	9	4	8	3	33112.900	33112.930	-.030
29	10	4	9	3	33113.550	33113.607	-.057
30	8	6	7	5	33115.100	33114.991	.109
31	8	8	7	7	33116.050	33116.145	-.095
32	9	8	8	7	33116.900	33116.819	.081
33	10	8	9	7	33117.600	33117.497	.103
34	11	8	10	7	33118.400	33118.178	.222
35	13	8	12	7	33119.500	33119.550	-.050
36	15	8	14	7	33120.990	33120.934	.057
37	10	10	9	9	33117.200	33117.182	.018
38	11	10	10	9	33117.800	33117.863	-.063
39	13	10	12	9	33119.200	33119.234	-.034
40	12	12	11	11	33116.900	33116.892	.008
41	13	12	12	11	33117.600	33117.577	.023
42	15	12	14	11	33118.800	33118.958	-.158
43	16	12	15	11	33119.750	33119.652	.098
44	17	12	16	11	33120.350	33120.351	-.000
45	18	12	17	11	33120.990	33121.052	-.062

Table 8. (Continued).

* * * * * * * * P BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
0	0	1	1	33096.06	.00	.00
1	0	2	1	33095.33	.00	.00
2	0	3	1	33094.93	.00	.00
3	0	4	1	33093.90	.00	.00
4	0	5	1	33093.92	.00	.00
5	0	6	1	33092.41	.00	.00
6	0	7	1	33093.05	.00	.00
7	0	8	1	33090.85	.00	.00
8	0	9	1	33092.33	.00	.00
9	0	10	1	33089.27	.00	.00
10	0	11	1	33091.77	.00	.00
2	2	3	3	33087.12	.00	.00
3	2	4	3	33086.49	.00	.00
4	2	5	3	33085.87	.00	.00
5	2	6	3	33085.25	.00	.00
6	2	7	3	33084.63	.00	.00
7	2	8	3	33084.01	.00	.00
8	2	9	3	33083.40	.00	.00
9	2	10	3	33082.76	.00	.00
10	2	11	3	33082.17	.00	.00
11	2	12	3	33081.48	.00	.00
12	2	13	3	33080.94	.00	.00
4	4	5	5	33076.58	33076.57	-.01
5	4	6	5	33075.97	.00	.00
6	4	7	5	33075.35	.00	.00
7	4	8	5	33074.74	.00	.00
8	4	9	5	33074.13	.00	.00
9	4	10	5	33073.53	.00	.00
10	4	11	5	33072.92	.00	.00
11	4	12	5	33072.32	.00	.00
12	4	13	5	33071.72	.00	.00
13	4	14	5	33071.12	.00	.00
14	4	15	5	33070.52	.00	.00
6	6	7	7	33064.50	33064.87	.37
7	6	8	7	33063.89	.00	.00
8	6	9	7	33063.29	33063.20	-.09
9	6	10	7	33062.68	.00	.00
10	6	11	7	33062.08	.00	.00
11	6	12	7	33061.48	.00	.00
12	6	13	7	33060.89	.00	.00
13	6	14	7	33060.30	.00	.00
14	6	15	7	33059.71	.00	.00
15	6	16	7	33059.12	.00	.00
16	6	17	7	33058.53	.00	.00
8	8	9	9	33050.97	33050.65	-.32
9	8	10	9	33050.37	33050.10	-.27
10	8	11	9	33049.77	33049.60	-.17

Table 8. (Continued).

11	8	12	9	33049.17	.00	.00
12	8	13	9	33048.57	.00	.00
13	8	14	9	33047.98	.00	.00
14	8	15	9	33047.39	.00	.00
15	8	16	9	33046.81	.00	.00
16	8	17	9	33046.23	.00	.00
17	8	18	9	33045.65	.00	.00
18	8	19	9	33045.07	.00	.00
10	10	11	11	33036.11	33036.28	.17
11	10	12	11	33035.51	33035.78	.27
12	10	13	11	33034.91	33034.9[illegible]	.08
13	10	14	11	33034.32	33034.37	.05
14	10	15	11	33033.73	.00	.00
15	10	16	11	3303[illegible].14	.00	.00
16	10	17	11	33032.56	.00	.00
17	10	18	11	33031.98	.00	.00
18	10	19	11	33031.40	.00	.00
19	10	20	11	33030.83	.00	.00
20	10	21	11	33030.25	.00	.00
12	12	13	13	33020.08	33020.03	-.05
13	12	14	13	33019.48	33019.30	-.18
14	12	15	13	33018.89	33018.90	.01
15	12	16	13	33018.30	.00	.00
16	12	17	13	33017.71	33017.72	.01
17	12	18	13	33017.12	33017.15	.03
18	12	19	13	33016.54	33016.58	.04
19	12	20	13	33015.96	.00	.00
20	12	21	13	33015.39	33015.30	-.09
21	12	22	13	33014.81	.00	.00
22	12	23	13	33014.24	.00	.00
14	14	15	15	33003.06	33002.99	-.07
15	14	16	15	33002.47	33002.50	.03
16	14	17	15	33001.87	33001.99	.12
17	14	18	15	33001.28	33001.29	.01
18	14	19	15	33000.69	33000.68	-.01
19	14	20	15	33000.11	.00	.00
20	14	21	15	32999.53	.00	.00
21	14	22	15	32998.95	.00	.00
22	14	23	15	32998.37	.00	.00
23	14	24	15	32997.80	.00	.00
24	14	25	15	32997.23	.00	.00
16	16	17	17	32985.28	.00	.00
17	16	18	17	32984.69	.00	.00
18	16	19	17	32984.09	.00	.00
19	16	20	17	32983.50	.00	.00
20	16	21	17	32982.91	.00	.00
21	16	22	17	32982.32	.00	.00
22	16	23	17	32981.73	.00	.00
23	16	24	17	32981.15	.00	.00
24	16	25	17	32980.57	.00	.00
25	16	26	17	32980.00	.00	.00
26	16	27	17	32979.42	.00	.00

Table 8. (Continued).

18	18	19	19	32966.99	.00	.00
19	18	20	19	32966.39	.00	.00
20	18	21	19	32965.79	.00	.00
21	18	22	19	32965.19	.00	.00
22	18	23	19	32964.60	.00	.00
23	18	24	19	32964.00	.00	.00
24	18	25	19	32963.41	.00	.00
25	18	26	19	32962.82	.00	.00
26	18	27	19	32962.24	.00	.00
27	18	28	19	32961.65	.00	.00
28	18	29	19	32961.07	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
2	2	1	1	33103.99	.00	.00
3	2	2	1	33104.54	.00	.00
4	2	3	1	33105.43	.00	.00
5	2	4	1	33105.69	.00	.00
6	2	5	1	33106.99	.00	.00
7	2	6	1	33106.76	.00	.00
8	2	7	1	33108.69	.00	.00
9	2	8	1	33107.78	.00	.00
10	2	9	1	33110.54	.00	.00
11	2	10	1	33108.76	.00	.00
12	2	11	1	33112.54	.00	.00
4	4	3	3	33109.61	33109.40	-.21
5	4	4	3	33110.27	33110.30	.03
6	4	5	3	33110.94	33110.90	-.04
7	4	6	3	33111.60	33111.60	.00
8	4	7	3	33112.27	33112.40	.13
9	4	8	3	33112.93	33112.90	-.03
10	4	9	3	33113.61	33113.55	-.06
11	4	10	3	33114.25	.00	.00
12	4	11	3	33114.95	.00	.00
13	4	12	3	33115.54	.00	.00
14	4	13	3	33116.29	.00	.00
6	6	5	5	33113.65	.00	.00
7	6	6	5	33114.32	.00	.00
8	6	7	5	33114.99	33115.10	.11
9	6	8	5	33115.67	.00	.00
10	6	9	5	33116.34	.00	.00
11	6	10	5	33117.02	.00	.00
12	6	11	5	33117.70	.00	.00
13	6	12	5	33118.39	.00	.00
14	6	13	5	33119.07	.00	.00
15	6	14	5	33119.75	.00	.00
16	6	15	5	33120.44	.00	.00
8	8	7	7	33116.14	33116.05	-.09
9	8	8	7	33116.82	33116.90	.08
10	8	9	7	33117.50	33117.60	.10

Table 8. (Continued).

11	8	10	7	33118.18	33118.40	.22
12	8	11	7	33118.86	.00	.00
13	8	12	7	33119.55	33119.50	-.05
14	8	13	7	33120.24	.00	.00
15	8	14	7	33120.93	33120.99	.06
16	8	15	7	33121.63	.00	.00
17	8	16	7	33122.33	.00	.00
18	8	17	7	33123.02	.00	.00

10	10	9	9	33117.18	33117.20	.02
11	10	10	9	33117.86	33117.80	-.06
12	10	11	9	33118.55	.00	.00
13	10	12	9	33119.23	33119.20	-.03
14	10	13	9	33119.92	.00	.00
15	10	14	9	33120.62	.00	.00
16	10	15	9	33121.32	.00	.00
17	10	16	9	33122.02	.00	.00
18	10	17	9	33122.72	.00	.00
19	10	18	9	33123.42	.00	.00
20	10	19	9	33124.13	.00	.00

12	12	11	11	33116.89	33116.90	.01
13	12	12	11	33117.58	33117.60	.02
14	12	13	11	33118.27	.00	.00
15	12	14	11	33118.96	33118.80	-.16
16	12	15	11	33119.65	33119.75	.10
17	12	16	11	33120.35	33120.35	-.00
18	12	17	11	33121.05	33120.99	-.06
19	12	18	11	33121.76	.00	.00
20	12	19	11	33122.46	.00	.00
21	12	20	11	33123.17	.00	.00
22	12	21	11	33123.89	.00	.00

14	14	13	13	33115.43	.00	.00
15	14	14	13	33116.12	.00	.00
16	14	15	13	33116.81	.00	.00
17	14	16	13	33117.50	.00	.00
18	14	17	13	33118.20	.00	.00
19	14	18	13	33118.90	.00	.00
20	14	19	13	33119.60	.00	.00
21	14	20	13	33120.31	.00	.00
22	14	21	13	33121.02	.00	.00
23	14	22	13	33121.73	.00	.00
24	14	23	13	33122.45	.00	.00

16	16	15	15	33112.99	.00	.00
17	16	16	15	33113.68	.00	.00
18	16	17	15	33114.37	.00	.00
19	16	18	15	33115.06	.00	.00
20	16	19	15	33115.76	.00	.00
21	16	20	15	33116.46	.00	.00
22	16	21	15	33117.16	.00	.00
23	16	22	15	33117.87	.00	.00
24	16	23	15	33118.58	.00	.00
25	16	24	15	33119.29	.00	.00
26	16	25	15	33120.00	.00	.00

Table 8. (Continued).

18	18	17	17	33109.78	.00	.00
19	18	18	17	33110.47	.00	.00
20	18	19	17	33111.16	.00	.00
21	18	20	17	33111.85	.00	.00
22	18	21	17	33112.54	.00	.00
23	18	22	17	33113.24	.00	.00
24	18	23	17	33113.94	.00	.00
25	18	24	17	33114.64	.00	.00
26	18	25	17	33115.35	.00	.00
27	18	26	17	33116.06	.00	.00
28	18	27	17	33116.77	.00	.00
20	20	19	19	33106.06	.00	.00
21	20	20	19	33106.74	.00	.00
22	20	21	19	33107.43	.00	.00
23	20	22	19	33108.11	.00	.00
24	20	23	19	33108.80	.00	.00
25	20	24	19	33109.50	.00	.00
26	20	25	19	33110.19	.00	.00
27	20	26	19	33110.89	.00	.00
28	20	27	19	33111.58	.00	.00
29	20	28	19	33112.29	.00	.00
30	20	29	19	33112.99	.00	.00

Table 9. Observed and Calculated Transition Frequencies in cm^{-1} for the G Band of SO_2^{16}.

BAND ORIGIN AT 33325.716 CM-1.
B= .321439
A-C= 1.527727
DK= .000000000000
DJK= .000000000000
DJ= .000000000000
ROOT MEAN SQUARE DEVIATION= .1259 CM-1 FOR 73 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	3	3	4	4	33309.850	33309.630	.220
2	4	3	5	4	33309.000	33309.010	-.010
3	5	3	6	4	33308.150	33308.394	-.244
4	6	3	7	4	33307.720	33307.781	-.061
5	7	3	8	4	33306.950	33307.171	-.221
6	8	3	9	4	33306.400	33306.564	-.165
7	9	3	10	4	33305.850	33305.958	-.108
8	5	5	6	6	33298.850	33298.759	.091
9	6	5	7	6	33298.100	33298.148	-.048
10	7	5	8	6	33297.700	33297.541	.159
11	8	5	9	6	33297.000	33296.937	.063
12	9	5	10	6	33296.290	33296.337	-.047
13	10	5	11	6	33295.950	33295.740	.210
14	11	5	12	6	33295.190	33295.146	.043
15	8	7	9	8	33285.980	33286.003	-.023
16	9	7	10	8	33285.420	33285.403	.017
17	10	7	11	8	33284.800	33284.808	-.008
18	11	7	12	8	33284.300	33284.215	.084
19	12	7	13	8	33283.450	33283.626	-.176
20	13	7	14	8	33283.000	33283.041	-.041
21	9	9	10	10	33273.250	33273.282	-.032
22	10	9	11	10	33272.750	33272.685	.065
23	11	9	12	10	33272.220	33272.091	.129
24	12	9	13	10	33271.590	33271.501	.088
25	13	9	14	10	33271.000	33270.915	.085
26	14	9	15	10	33270.550	33270.333	.217
27	15	9	16	10	33269.620	33269.753	-.133
28	11	11	12	12	33258.810	33258.927	-.117
29	12	11	13	12	33258.290	33258.334	-.044
30	15	11	16	12	33256.590	33256.577	.013
31	16	11	17	12	33256.000	33255.999	.001
32	17	11	18	12	33255.300	33255.424	-.124
33	18	11	19	12	33254.980	33254.852	.128
34	14	13	15	14	33242.910	33243.123	-.212
35	15	13	16	14	33242.500	33242.536	-.036
36	16	13	17	14	33242.100	33241.952	.148
37	3	3	2	2	33334.970	33334.576	.394
38	4	3	3	2	33335.410	33335.236	.174
39	5	3	4	2	33335.640	33335.883	-.243
40	6	3	5	2	33336.410	33336.571	-.161
41	7	3	6	2	33336.920	33337.173	-.253
42	8	3	7	2	33337.900	33337.938	-.039
43	9	3	8	2	33338.290	33338.408	-.118
44	10	3	9	2	33339.420	33339.347	.073
45	11	3	10	2	33339.600	33339.550	.050
46	12	3	11	2	33340.790	33340.810	-.020
47	5	5	4	4	33340.020	33339.860	.160
48	6	5	5	4	33340.390	33340.526	-.136
49	7	5	6	4	33341.250	33341.195	.055
50	8	5	7	4	33341.990	33341.869	.122

Table 9. (Continued).

51	9	5	8	4	33342.600	33342.544	.056
52	10	5	9	4	33343.350	33343.223	.127
53	11	5	10	4	33343.910	33343.903	.007
54	12	5	11	4	33344.630	33344.584	.045
55	13	5	12	4	33345.300	33345.264	.036
56	14	5	13	4	33345.900	33345.948	-.048
57	15	5	14	4	33346.600	33346.621	-.021
58	8	7	7	6	33344.400	33344.457	-.057
59	9	7	8	6	33344.950	33345.136	-.186
60	10	7	9	6	33345.750	33345.818	-.068
61	11	7	10	6	33346.550	33346.503	.046
62	12	7	11	6	33347.100	33347.192	-.092
63	13	7	12	6	33347.900	33347.884	.016
64	9	9	8	8	33346.500	33346.423	.077
65	10	9	9	8	33347.150	33347.105	.044
66	11	9	10	8	33347.970	33347.792	.179
67	12	9	11	8	33348.550	33348.481	.068
68	14	9	13	8	33350.000	33349.872	.128
69	15	9	14	8	33350.400	33350.572	-.172
70	11	11	10	10	33347.750	33347.893	-.143
71	12	11	11	10	33348.550	33348.581	-.031
72	15	11	14	10	33350.680	33350.668	.012
73	16	11	15	10	33351.400	33351.372	.028

Table 9. (Continued).

* * * * * * * *				P BRANCH * * * * * * * *		
J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	2	2	33319.14	.00	.00
2	1	3	2	33318.51	.00	.00
3	1	4	2	33317.88	.0	.0
4	1	5	2	33317.28	.00	.00
5	1	6	2	33316.59	.00	.00
6	1	7	2	33316.07	.00	.00
7	1	8	2	33315.26	.00	.00
8	1	9	2	33314.91	.00	.00
9	1	10	2	33313.83	.00	.00
10	1	11	2	33313.80	.00	.00
11	1	12	2	33312.28	.00	.00
3	3	4	4	33309.63	33309.85	.22
4	3	5	4	33309.01	33309.00	-.01
5	3	6	4	33308.39	33308.15	-.24
6	3	7	4	33307.78	33307.72	-.06
7	3	8	4	33307.17	33306.95	-.22
8	3	9	4	33306.56	33306.40	-.16
9	3	10	4	33305.96	33305.85	-.11
10	3	11	4	33305.35	.00	.00
11	3	12	4	33304.75	.00	.00
12	3	13	4	33304.15	.00	.00
13	3	14	4	33303.53	.00	.00
5	5	6	6	33298.76	33298.85	.09
6	5	7	6	33298.15	33298.10	-.05
7	5	8	6	33297.54	33297.70	.16
8	5	9	6	33296.94	33297.00	.06
9	5	10	6	33296.34	33296.29	-.05
10	5	11	6	33295.74	33295.95	.21
11	5	12	6	33295.15	33295.19	.04
12	5	13	6	33294.56	.00	.00
13	5	14	6	33293.97	.00	.00
14	5	15	6	33293.38	.00	.00
15	5	16	6	33292.79	.00	.00
7	7	8	8	33286.61	.00	.00
8	7	9	8	33286.00	33285.98	-.02
9	7	10	8	33285.40	33285.42	.02
10	7	11	8	33284.81	33284.80	-.01
11	7	12	8	33284.22	33284.30	.08
12	7	13	8	33283.63	33283.45	-.18
13	7	14	8	33283.04	33283.00	-.04
14	7	15	8	33282.46	.00	.00
15	7	16	8	33281.88	.00	.00
16	7	17	8	33281.30	.00	.00
17	7	18	8	33280.73	.00	.00
9	9	10	10	33273.28	33273.25	-.03
10	9	11	10	33272.69	33272.75	.06
11	9	12	10	33272.09	33272.22	.13
12	9	13	10	33271.50	33271.59	.09
13	9	14	10	33270.92	33271.00	.08
14	9	15	10	33270.33	33270.55	.22
15	9	16	10	33269.75	33269.62	-.13
16	9	17	10	33269.18	.00	.00

Table 9. (Continued).

17	9	18	10	33268.61	.00	.00
18	9	19	10	33268.04	.00	.00
19	9	20	10	33267.47	.00	.00
11	11	12	12	33258.93	33258.81	-.12
12	11	13	12	33258.33	33258.29	-.04
13	11	14	12	33257.74	.00	.00
14	11	15	12	33257.16	.00	.00
15	11	16	12	33256.58	33256.59	.01
16	11	17	12	33256.00	33256.00	.00
17	11	18	12	33255.42	33255.30	-.12
18	11	19	12	33254.85	33254.98	.13
19	11	20	12	33254.28	.00	.00
20	11	21	12	33253.72	.00	.00
21	11	22	12	33253.16	.00	.00
13	13	14	14	33243.71	.00	.00
14	13	15	14	33243.12	33242.91	-.21
15	13	16	14	33242.54	33242.50	-.04
16	13	17	14	33241.95	33242.10	.15
17	13	18	14	33241.37	.00	.00
18	13	19	14	33240.80	.00	.00
19	13	20	14	33240.2	.00	.00
20	13	21	14	33239.65	.00	.00
21	13	22	14	33239.09	.00	.00
22	13	23	14	33238.52	.00	.00
23	13	24	14	33237.96	.00	.00
15	15	16	16	33227.84	.00	.00
16	15	17	16	33227.25	.00	.00
17	15	18	16	33226.67	.00	.00
18	15	19	16	33226.08	.00	.00
19	15	20	16	33225.50	.00	.00
20	15	21	16	33224.93	.00	.00
21	15	22	16	33224.35	.00	.00
22	15	23	16	33223.78	.00	.00
23	15	24	16	33223.21	.00	.00
24	15	25	16	33222.65	.00	.00
25	15	26	16	33222.09	.00	.00
17	17	18	18	33211.56	.00	.00
18	17	19	18	33210.96	.00	.00
19	17	20	18	33210.37	.00	.00
20	17	21	18	33209.79	.00	.00
21	17	22	18	33209.21	.00	.00
22	17	23	18	33208.62	.00	.00
23	17	24	18	33208.05	.00	.00
24	17	25	18	33207.47	.00	.00
25	17	26	18	33206.90	.00	.00
26	17	27	18	33206.33	.00	.00
27	17	28	18	33205.77	.00	.00
19	19	20	20	33195.12	.00	.00
20	19	21	20	33194.52	.00	.00
21	19	22	20	33193.92	.00	.00
22	19	23	20	33193.33	.00	.00
23	19	24	20	33192.74	.00	.00
24	19	25	20	33192.16	.00	.00
25	19	26	20	33191.57	.00	.00
26	19	27	20	33190.99	.00	.00

Table 9. (Continued).

27	19	28	20	33190.41	.00	.00
28	19	29	20	33189.83	.00	.00
29	19	30	20	33189.26	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	0	0	33327.89	.00	.00
2	1	1	0	33329.17	.00	.00
3	1	2	0	33329.19	.00	.00
4	1	3	0	33333.67	.00	.00
5	1	4	0	33330.53	.00	.00
6	1	5	0	33340.74	.00	.00
7	1	6	0	33331.93	.00	.00
8	1	7	0	33350.39	.00	.00
9	1	8	0	33333.45	.00	.00
10	1	9	0	33362.60	.00	.00
11	1	10	0	33335.13	.00	.00
3	3	2	2	33334.58	33334.97	.39
4	3	3	2	33335.24	33335.41	.17
5	3	4	2	33335.88	33335.64	-.24
6	3	5	2	33336.57	33336.41	-.16
7	3	6	2	33337.17	33336.92	-.25
8	3	7	2	33337.94	33337.90	-.04
9	3	8	2	33338.41	33338.29	-.12
10	3	9	2	33339.35	33339.42	.07
11	3	10	2	33339.55	33339.60	.05
12	3	11	2	33340.81	33340.79	-.02
13	3	12	2	33340.57	.00	.00
5	5	4	4	33339.86	33340.02	.16
6	5	5	4	33340.53	33340.39	-.14
7	5	6	4	33341.20	33341.25	.05
8	5	7	4	33341.87	33341.99	.12
9	5	8	4	33342.54	33342.60	.06
10	5	9	4	33343.22	33343.35	.13
11	5	10	4	33343.90	33343.91	.01
12	5	11	4	33344.58	33344.63	.05
13	5	12	4	33345.26	33345.30	.04
14	5	13	4	33345.95	33345.90	-.05
15	5	14	4	33346.62	33346.60	-.02
7	7	6	6	33343.78	.00	.00
8	7	7	6	33344.46	33344.40	-.06
9	7	8	6	33345.14	33344.95	-.19
10	7	9	6	33345.82	33345.75	-.07
11	7	10	6	33346.50	33346.55	.05
12	7	11	6	33347.19	33347.10	-.09
13	7	12	6	33347.88	33347.90	.02
14	7	13	6	33348.58	.00	.00
15	7	14	6	33349.28	.00	.00
16	7	15	6	33349.97	.00	.00
17	7	16	6	33350.67	.00	.00
9	9	8	8	33346.42	33346.50	.08
10	9	9	8	33347.11	33347.15	.04
11	9	10	8	33347.79	33347.97	.18
12	9	11	8	33348.48	33348.55	.07
13	9	12	8	33349.18	.00	.00

Table 9. (Continued).

14	9	13	8	33349.87	33350.00	.13
15	9	14	8	33350.57	33350.40	-.17
16	9	15	8	33351.28	.00	.00
17	9	16	8	33351.98	.00	.00
18	9	17	8	33352.69	.00	.00
19	9	18	8	33353.40	.00	.00
11	11	10	10	33347.89	33347.75	-.14
12	11	11	10	33348.58	33348.55	-.03
13	11	12	10	33349.27	.00	.00
14	11	13	10	33349.97	.00	.00
15	11	14	10	33350.67	33350.68	.01
16	11	15	10	33351.37	33351.40	.03
17	11	16	10	33352.08	.00	.00
18	11	17	10	33352.79	.00	.00
19	11	18	10	33353.50	.00	.00
20	11	19	10	33354.22	.00	.00
21	11	20	10	33354.94	.00	.00
13	13	12	12	33348.33	.00	.00
14	13	13	12	33349.02	.00	.00
15	13	14	12	33349.72	.00	.00
16	13	15	12	33350.42	.00	.00
17	13	16	12	33351.12	.00	.00
18	13	17	12	33351.83	.00	.00
19	13	18	12	33352.54	.00	.00
20	13	19	12	33353.26	.00	.00
21	13	20	12	33353.97	.00	.00
22	13	21	12	33354.69	.00	.00
23	13	22	12	33355.42	.00	.00
15	15	14	14	33347.91	.00	.00
16	15	15	14	33348.60	.00	.00
17	15	16	14	33349.30	.00	.00
18	15	17	14	33350.01	.00	.00
19	15	18	14	33350.71	.00	.00
20	15	19	14	33351.42	.00	.00
21	15	20	14	33352.13	.00	.00
22	15	21	14	33352.85	.00	.00
23	15	22	14	33353.57	.00	.00
24	15	23	14	33354.29	.00	.00
25	15	24	14	33355.02	.00	.00
17	17	16	16	33346.83	.00	.00
18	17	17	16	33347.53	.00	.00
19	17	18	16	33348.23	.00	.00
20	17	19	16	33348.93	.00	.00
21	17	20	16	33349.64	.00	.00
22	17	21	16	33350.35	.00	.00
23	17	22	16	33351.06	.00	.00
24	17	23	16	33351.77	.00	.00
25	17	24	16	33352.49	.00	.00
26	17	25	16	33353.21	.00	.00
27	17	26	16	33353.94	.00	.00
19	19	18	18	33345.34	.00	.00
20	19	19	18	33346.03	.00	.00
21	19	20	18	33346.73	.00	.00
22	19	21	18	33347.43	.00	.00
23	19	22	18	33348.13	.00	.00

Table 9. (Continued).

24	19	23	18	33348.84	.00	.00
25	19	24	18	33349.55	.00	.00
26	19	25	18	33350.26	.00	.00
27	19	26	18	33350.97	.00	.00
28	19	27	18	33351.69	.00	.00
29	19	28	18	33352.41	.00	.00

Table 10. Observed and Calculated Transition Frequencies in cm^{-1} for the A Band of SO_2^{18}.

BAND ORIGIN AT 31817.957 CM-1.
B= .288746
A-C= 1.433677
DK= .000000000000
DJK= .000000000000
DJ= .000000000000
ROOT MEAN SQUARE DEVIATION= .1142 CM-1 FOR 79 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	3	1	4	2	31810.500	31810.635	-.135
2	4	1	5	2	31810.020	31810.114	-.094
3	5	1	6	2	31809.550	31809.532	.018
4	6	1	7	2	31809.030	31809.079	-.049
5	7	1	8	2	31808.500	31808.407	.093
6	3	3	4	4	31802.330	31802.560	-.230
7	4	3	5	4	31802.050	31802.023	.027
8	7	3	8	4	31800.550	31800.455	.095
9	8	3	9	4	31800.150	31799.946	.204
10	13	3	14	4	31797.510	31797.469	.041
11	7	7	8	8	31779.600	31779.596	.004
12	8	7	9	8	31779.050	31779.092	-.042
13	9	7	10	8	31778.500	31778.595	-.095
14	10	7	11	8	31778.050	31778.105	-.055
15	11	7	12	8	31777.600	31777.624	-.024
16	12	7	13	8	31777.000	31777.149	-.149
17	13	7	14	8	31776.500	31776.682	-.182
18	14	7	15	8	31776.100	31776.221	-.121
19	15	7	16	8	31775.780	31775.768	.012
20	16	7	17	8	31775.400	31775.321	.079
21	11	11	12	12	31750.600	31750.497	.103
22	12	11	13	12	31750.100	31750.025	.075
23	13	11	14	12	31749.500	31749.562	-.062
24	14	11	15	12	31749.080	31749.105	-.025
25	15	11	16	12	31748.680	31748.656	.023
26	16	11	17	12	31748.200	31748.215	-.015
27	18	11	19	12	31747.420	31747.355	.065
28	21	11	22	12	31746.120	31746.118	.002
29	13	13	14	14	31733.700	31733.647	.052
30	14	13	15	14	31733.300	31733.192	.108
31	15	13	16	14	31732.900	31732.744	.156
32	17	13	18	14	31731.950	31731.872	.078
33	22	13	23	14	31729.900	31729.823	.077
34	23	13	24	14	31729.210	31729.434	-.224
35	13	9	14	10	31763.990	31763.907	.083
36	15	9	16	10	31763.080	31762.999	.081
37	16	9	17	10	31762.480	31762.555	-.075
38	18	9	19	10	31761.690	31761.689	.000
39	19	9	20	10	31761.400	31761.267	.133
40	3	1	2	0	31821.000	31821.149	-.149
41	5	1	4	0	31822.480	31822.375	.105
42	7	1	6	0	31823.800	31823.669	.131
43	3	3	2	2	31826.190	31826.099	.091
44	4	3	3	2	31826.720	31826.702	.018
45	5	3	4	2	31827.200	31827.302	-.102
46	6	3	5	2	31827.950	31827.936	.014
47	7	3	6	2	31828.560	31828.509	.051
48	8	3	7	2	31829.100	31829.211	-.111
49	9	3	8	2	31829.810	31829.694	.116
50	5	5	4	4	31830.610	31830.697	-.086

Table 10. (Continued).

51	6	5	5	4	31831.200	31831.314	-.115
52	7	5	6	4	31832.030	31831.940	.090
53	8	5	7	4	31832.600	31832.572	.028
54	9	5	8	4	31833.300	31833.211	.089
55	11	5	10	4	31834.620	31834.508	.113
56	7	7	6	6	31833.700	31833.760	-.061
57	8	7	7	6	31834.290	31834.395	-.105
58	9	7	8	6	31835.100	31835.037	.063
59	10	7	9	6	31835.790	31835.686	.104
60	11	7	10	6	31836.350	31836.342	.008
61	12	7	11	6	31837.150	31837.006	.144
62	13	7	12	6	31837.610	31837.676	-.066
63	9	9	8	8	31835.100	31835.291	-.191
64	10	9	9	8	31835.790	31835.941	-.151
65	12	9	11	8	31837.300	31837.266	.034
66	13	9	12	8	31837.910	31837.939	-.029
67	14	9	13	8	31838.650	31838.619	.031
68	11	11	10	10	31835.790	31835.288	.502
69	12	11	11	10	31835.790	31835.955	-.165
70	14	11	13	10	31837.300	31837.312	-.011
71	15	11	14	10	31837.900	31838.001	-.102
72	16	11	15	10	31838.800	31838.699	.101
73	17	11	16	10	31839.500	31839.403	.097
74	14	13	13	12	31834.290	31834.434	-.144
75	15	13	14	12	31835.100	31835.125	-.025
76	16	13	15	12	31835.790	31835.824	-.034
77	17	13	16	12	31836.400	31836.530	-.130
78	18	13	17	12	31837.150	31837.244	-.094
79	19	13	18	12	31837.880	31837.965	-.085

Table 10. (Continued).

* * * * * * * * P BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	2	2	31811.74	.00	.00
2	1	3	2	31811.19	.00	.00
3	1	4	2	31810.63	31810.50	-.13
4	1	5	2	31810.11	31810.02	-.09
5	1	6	2	31809.53	31809.55	.02
6	1	7	2	31809.08	31809.03	-.05
7	1	8	2	31808.41	31808.50	.09
8	1	9	2	31808.09	.00	.00
9	1	10	2	31807.23	.00	.00
10	1	11	2	31807.16	.00	.00
11	1	12	2	31805.97	.00	.00
3	3	4	4	31802.56	31802.33	-.23
4	3	5	4	31802.02	31802.05	.03
5	3	6	4	31801.49	.00	.00
6	3	7	4	31800.97	.00	.00
7	3	8	4	31800.46	31800.55	.09
8	3	9	4	31799.95	31800.15	.20
9	3	10	4	31799.44	.00	.00
10	3	11	4	31798.94	.00	.00
11	3	12	4	31798.45	.00	.00
12	3	13	4	31797.96	.00	.00
13	3	14	4	31797.47	31797.51	.04
5	5	6	6	31791.84	.00	.00
6	5	7	6	31791.32	.00	.00
7	5	8	6	31790.81	.00	.00
8	5	9	6	31790.31	.00	.00
9	5	10	6	31789.81	.00	.00
10	5	11	6	31789.32	.00	.00
11	5	12	6	31788.83	.00	.00
12	5	13	6	31788.35	.00	.00
13	5	14	6	31787.88	.00	.00
14	5	15	6	31787.41	.00	.00
15	5	16	6	31786.95	.00	.00
7	7	8	8	31779.60	31779.60	.00
8	7	9	8	31779.09	31779.05	-.04
9	7	10	8	31778.59	31778.50	-.09
10	7	11	8	31778.11	31778.05	-.06
11	7	12	8	31777.62	31777.60	-.02
12	7	13	8	31777.15	31777.00	-.15
13	7	14	8	31776.68	31776.50	-.18
14	7	15	8	31776.22	31776.10	-.12
15	7	16	8	31775.77	31775.78	.01
16	7	17	8	31775.32	31775.40	.08
17	7	18	8	31774.88	.00	.00
9	9	10	10	31765.81	.00	.00
10	9	11	10	31765.33	.00	.00
11	9	12	10	31764.84	.00	.00
12	9	13	10	31764.37	.00	.00
13	9	14	10	31763.91	31763.99	.08
14	9	15	10	31763.45	.00	.00
15	9	16	10	31763.00	31763.08	.08

Table 10. (Continued).

16	9	17	10	31762.56	31762.48	-.08
17	9	18	10	31762.12	.00	.00
18	9	19	10	31761.69	31761.69	.00
19	9	20	10	31761.27	31761.40	.13
11	11	12	12	31750.50	31750.60	.10
12	11	13	12	31750.03	31750.10	.07
13	11	14	12	31749.56	31749.50	-.06
14	11	15	12	31749.11	31749.08	-.03
15	11	16	12	31748.66	31748.68	.02
16	11	17	12	31748.22	31748.20	-.02
17	11	18	12	31747.78	.00	.00
18	11	19	12	31747.35	31747.42	.06
19	11	20	12	31746.94	.00	.00
20	11	21	12	31746.52	.00	.00
21	11	22	12	31746.12	31746.12	.00
13	13	14	14	31733.65	31733.70	.05
14	13	15	14	31733.19	31733.30	.11
15	13	16	14	31732.74	31732.90	.16
16	13	17	14	31732.30	.00	.00
17	13	18	14	31731.87	31731.95	.08
18	13	19	14	31731.45	.00	.00
19	13	20	14	31731.03	.00	.00
20	13	21	14	31730.62	.00	.00
21	13	22	14	31730.22	.00	.00
22	13	23	14	31729.82	31729.90	.08
23	13	24	14	31729.43	31729.21	-.22
15	15	16	16	31715.26	.00	.00
16	15	17	16	31714.82	.00	.00
17	15	18	16	31714.39	.00	.00
18	15	19	16	31713.97	.00	.00
19	15	20	16	31713.55	.00	.00
20	15	21	16	31713.15	.00	.00
21	15	22	16	31712.75	.00	.00
22	15	23	16	31712.35	.00	.00
23	15	24	16	31711.97	.00	.00
24	15	25	16	31711.59	.00	.00
25	15	26	16	31711.22	.00	.00
17	17	18	18	31695.35	.00	.00
18	17	19	18	31694.92	.00	.00
19	17	20	18	31694.51	.00	.00
20	17	21	18	31694.10	.00	.00
21	17	22	18	31693.70	.00	.00
22	17	23	18	31693.31	.00	.00
23	17	24	18	31692.93	.00	.00
24	17	25	18	31692.55	.00	.00
25	17	26	18	31692.18	.00	.00
26	17	27	18	31691.82	.00	.00
27	17	28	18	31691.46	.00	.00
19	19	20	20	31673.90	.00	.00
20	19	21	20	31673.49	.00	.00
21	19	22	20	31673.09	.00	.00
22	19	23	20	31672.70	.00	.00
23	19	24	20	31672.32	.00	.00
24	19	25	20	31671.94	.00	.00
25	19	26	20	31671.57	.00	.00

Table 10. (Continued).

26	19	27	20	31671.21	.00	.00
27	19	28	20	31670.86	.00	.00
28	19	29	20	31670.52	.00	.00
29	19	30	20	31670.18	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	0	0	31819.97	.00	.00
2	1	1	0	31821.12	.00	.00
3	1	2	0	31821.15	31821.00	-.15
4	1	3	0	31825.17	.00	.00
5	1	4	0	31822.37	31822.48	.10
6	1	5	0	31831.52	.00	.00
7	1	6	0	31823.67	31823.80	.13
8	1	7	0	31840.18	.00	.00
9	1	8	0	31825.06	.00	.00
10	1	9	0	31851.15	.00	.00
11	1	10	0	31826.60	.00	.00
3	3	2	2	31826.10	31826.19	.09
4	3	3	2	31826.70	31826.72	.02
5	3	4	2	31827.30	31827.20	-.10
6	3	5	2	31827.94	31827.95	.01
7	3	6	2	31828.51	31828.56	.05
8	3	7	2	31829.21	31829.10	-.11
9	3	8	2	31829.69	31829.81	.12
10	3	9	2	31830.53	.00	.00
11	3	10	2	31830.82	.00	.00
12	3	11	2	31831.92	.00	.00
13	3	12	2	31831.87	.00	.00
5	5	4	4	31830.70	31830.61	-.09
6	5	5	4	31831.31	31831.20	-.11
7	5	6	4	31831.94	31832.03	.09
8	5	7	4	31832.57	31832.60	.03
9	5	8	4	31833.21	31833.30	.09
10	5	9	4	31833.86	.00	.00
11	5	10	4	31834.51	31834.62	.11
12	5	11	4	31835.16	.00	.00
13	5	12	4	31835.82	.00	.00
14	5	13	4	31836.49	.00	.00
15	5	14	4	31837.16	.00	.00
7	7	6	6	31833.76	31833.70	-.06
8	7	7	6	31834.39	31834.29	-.10
9	7	8	6	31835.04	31835.10	.06
10	7	9	6	31835.69	31835.79	.10
11	7	10	6	31836.34	31836.35	.01
12	7	11	6	31837.01	31837.15	.14
13	7	12	6	31837.68	31837.61	-.07
14	7	13	6	31838.35	.00	.00
15	7	14	6	31839.04	.00	.00
16	7	15	6	31839.72	.00	.00
17	7	16	6	31840.42	.00	.00
9	9	8	8	31835.29	31835.10	-.19
10	9	9	8	31835.94	31835.79	-.15
11	9	10	8	31836.60	.00	.00
12	9	11	8	31837.27	31837.30	.03

Table 10. (Continued).

13	9	12	8	31837.94	31837.91	-.03
14	9	13	8	31838.62	31838.65	.03
15	9	14	8	31839.31	.00	.00
16	9	15	8	31840.00	.00	.00
17	9	16	8	31840.70	.00	.00
18	9	17	8	31841.41	.00	.00
19	9	18	8	31842.12	.00	.00
11	11	10	10	31835.29	31835.79	.50
12	11	11	10	31835.95	31835.79	-.16
13	11	12	10	31836.63	.00	.00
14	11	13	10	31837.31	31837.30	-.01
15	11	14	10	31838.00	31837.90	-.10
16	11	15	10	31838.70	31838.80	.10
17	11	16	10	31839.40	31839.50	.10
18	11	17	10	31840.11	.00	.00
19	11	18	10	31840.83	.00	.00
20	11	19	10	31841.56	.00	.00
21	11	20	10	31842.29	.00	.00
13	13	12	12	31833.75	.00	.00
14	13	13	12	31834.43	31834.29	-.14
15	13	14	12	31835.13	31835.10	-.03
16	13	15	12	31835.82	31835.79	-.03
17	13	16	12	31836.53	31836.40	-.13
18	13	17	12	31837.24	31837.15	-.09
19	13	18	12	31837.97	31837.88	-.09
20	13	19	12	31838.69	.00	.00
21	13	20	12	31839.43	.00	.00
22	13	21	12	31840.17	.00	.00
23	13	22	12	31840.92	.00	.00
15	15	14	14	31830.68	.00	.00
16	15	15	14	31831.38	.00	.00
17	15	16	14	31832.09	.00	.00
18	15	17	14	31832.80	.00	.00
19	15	18	14	31833.53	.00	.00
20	15	19	14	31834.26	.00	.00
21	15	20	14	31834.99	.00	.00
22	15	21	14	31835.74	.00	.00
23	15	22	14	31836.49	.00	.00
24	15	23	14	31837.25	.00	.00
25	15	24	14	31838.02	.00	.00
17	17	16	16	31826.08	.00	.00
18	17	17	16	31826.79	.00	.00
19	17	18	16	31827.52	.00	.00
20	17	19	16	31828.25	.00	.00
21	17	20	16	31828.99	.00	.00
22	17	21	16	31829.73	.00	.00
23	17	22	16	31830.49	.00	.00
24	17	23	16	31831.25	.00	.00
25	17	24	16	31832.02	.00	.00
26	17	25	16	31832.80	.00	.00
27	17	26	16	31833.58	.00	.00
19	19	18	18	31819.94	.00	.00
20	19	19	18	31820.67	.00	.00
21	19	20	18	31821.41	.00	.00
22	19	21	18	31822.16	.00	.00

Table 10. (Continued).

23	19	22	18	31822.91	.00	.00
24	19	23	18	31823.68	.00	.00
25	19	24	18	31824.45	.00	.00
26	19	25	18	31825.23	.00	.00
27	19	26	18	31826.01	.00	.00
28	19	27	18	31826.81	.00	.00
29	19	28	18	31827.61	.00	.00

Table 11. Observed and Calculated Transition Frequencies in cm^{-1} for the B Band of SO_2^{18}.

BAND ORIGIN AT 32049.940 CM-1.

B= .277497
A-C= 1.449490

DK= .000000000000
DJK= .000000000000
DJ= .000000000000
ROOT MEAN SQUARE DEVIATION= .1242 CM-1 FOR 74 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	2	2	3	3	32039.350	32039.322	.028
2	3	2	4	3	32038.900	32038.709	.191
3	4	2	5	3	32037.990	32038.081	-.091
4	5	2	6	3	32037.500	32037.436	.064
5	6	2	7	3	32036.620	32036.778	-.157
6	7	2	8	3	32036.150	32036.096	.053
7	4	4	5	5	32029.300	32029.406	-.105
8	5	4	6	5	32028.800	32028.764	.036
9	6	4	7	5	32028.110	32028.108	.002
10	7	4	8	5	32027.580	32027.436	.144
11	8	4	9	5	32026.900	32026.749	.151
12	9	4	10	5	32026.180	32026.046	.134
13	10	4	11	5	32025.210	32025.327	-.117
14	11	4	12	5	32024.610	32024.592	.018
15	6	6	7	7	32017.990	32017.992	-.002
16	7	6	8	7	32017.500	32017.322	.178
17	9	6	10	7	32016.000	32015.937	.063
18	10	6	11	7	32015.200	32015.222	-.022
19	11	6	12	7	32014.400	32014.492	-.092
20	12	6	13	7	32013.550	32013.746	-.196
21	13	6	14	7	32012.880	32012.984	-.104
22	14	6	15	7	32012.230	32012.206	.024
23	8	8	9	9	32005.250	32005.082	.168
24	9	8	10	9	32004.300	32004.383	-.083
25	10	8	11	9	32003.400	32003.669	-.270
26	11	8	12	9	32002.950	32002.941	.009
27	12	8	13	9	32002.130	32002.198	-.068
28	13	8	14	9	32001.500	32001.439	.061
29	14	8	15	9	32000.300	32000.665	-.365
30	10	10	11	11	31990.850	31990.674	.176
31	11	10	12	11	31990.050	31989.947	.104
32	12	10	13	11	31989.300	31989.204	.096
33	12	12	13	13	31974.620	31974.769	-.149
34	13	12	14	13	31973.960	31974.013	-.053
35	14	12	15	13	31973.210	31973.242	-.032
36	15	12	16	13	31972.210	31972.457	-.247
37	16	12	17	13	31971.820	31971.656	.164
38	17	12	18	13	31970.960	31970.841	.119
39	18	12	19	13	31970.200	31970.010	.189
40	19	12	20	13	31969.500	31969.165	.335
41	20	12	21	13	31968.200	31968.304	-.104
42	14	14	15	15	31957.410	31957.368	.042
43	15	14	16	15	31956.680	31956.583	.097
44	16	14	17	15	31955.900	31955.783	.116
45	17	14	18	15	31954.860	31954.969	-.109
46	4	4	3	3	32060.450	32060.601	-.151
47	5	4	4	3	32061.090	32061.098	-.008
48	6	4	5	3	32061.500	32061.580	-.080
49	7	4	6	3	32062.190	32062.045	.145
50	8	4	7	3	32062.500	32062.496	.004

Table 11. (Continued).

51	9	4	8	3	32063.030	32062.925	.105
52	10	4	9	3	32063.310	32063.347	-.037
53	6	6	5	5	32064.600	32064.500	.100
54	7	6	6	5	32064.990	32064.969	.021
55	8	6	7	5	32065.600	32065.422	.178
56	9	6	8	5	32065.700	32065.861	-.161
57	10	6	9	5	32066.320	32066.284	.036
58	10	8	9	7	32067.650	32067.768	-.118
59	11	8	10	7	32068.250	32068.178	.072
60	12	8	11	7	32068.500	32068.573	-.073
61	13	8	12	7	32069.000	32068.952	.048
62	14	8	13	7	32069.300	32069.316	-.016
63	10	10	9	9	32067.650	32067.808	-.158
64	11	10	10	9	32068.250	32068.219	.031
65	12	10	11	9	32068.500	32068.616	-.116
66	13	10	12	9	32069.000	32068.997	.003
67	12	12	11	11	32067.150	32067.216	-.066
68	13	12	12	11	32067.650	32067.599	.051
69	15	12	14	11	32068.250	32068.320	-.070
70	18	12	17	11	32069.300	32069.289	.011
71	14	14	13	13	32065.000	32065.128	-.128
72	15	14	14	13	32065.600	32065.482	.118
73	17	14	16	13	32066.150	32066.145	.005
74	18	14	17	13	32066.320	32066.455	-.135

Table 11. (Continued).

* * * * * * * * P BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
0	0	1	1	32047.76	.00	.00
1	0	2	1	32047.09	.00	.00
2	0	3	1	32046.69	.00	.00
3	0	4	1	32045.74	.00	.00
4	0	5	1	32045.65	.00	.00
5	0	6	1	32044.25	.00	.00
6	0	7	1	32044.65	.00	.00
7	0	8	1	32042.64	.00	.00
8	0	9	1	32043.70	.00	.00
9	0	10	1	32040.92	.00	.00
10	0	11	1	32042.82	.00	.00
2	2	3	3	32039.32	32039.35	.03
3	2	4	3	32038.71	32038.90	.19
4	2	5	3	32038.08	32037.99	-.09
5	2	6	3	32037.44	32037.50	.06
6	2	7	3	32036.78	32036.62	-.16
7	2	8	3	32036.10	32036.15	.05
8	2	9	3	32035.41	.00	.00
9	2	10	3	32034.68	.00	.00
10	2	11	3	32033.97	.00	.00
11	2	12	3	32033.17	.00	.00
12	2	13	3	32032.46	.00	.00
4	4	5	5	32029.41	32029.30	-.11
5	4	6	5	32028.76	32028.80	.04
6	4	7	5	32028.11	32028.11	.00
7	4	8	5	32027.44	32027.58	.14
8	4	9	5	32026.75	32026.90	.15
9	4	10	5	32026.05	32026.18	.13
10	4	11	5	32025.33	32025.21	-.12
11	4	12	5	32024.59	32024.61	.02
12	4	13	5	32023.84	.00	.00
13	4	14	5	32023.07	.00	.00
14	4	15	5	32022.28	.00	.00
6	6	7	7	32017.99	32017.99	-.00
7	6	8	7	32017.32	32017.50	.18
8	6	9	7	32016.64	.00	.00
9	6	10	7	32015.94	32016.00	.06
10	6	11	7	32015.22	32015.20	-.02
11	6	12	7	32014.49	32014.40	-.09
12	6	13	7	32013.75	32013.55	-.20
13	6	14	7	32012.98	32012.88	-.10
14	6	15	7	32012.21	32012.23	.02
15	6	16	7	32011.41	.00	.00
16	6	17	7	32010.60	.00	.00
8	8	9	9	32005.08	32005.25	.17
9	8	10	9	32004.38	32004.30	-.08
10	8	11	9	32003.67	32003.40	-.27

Table 11. (Continued).

11	8	12	9	32002.94	32002.95	.01
12	8	13	9	32002.20	32002.13	-.07
13	8	14	9	32001.44	32001.50	.06
14	8	15	9	32000.67	32000.30	-.36
15	8	16	9	31999.88	.00	.00
16	8	17	9	31999.07	.00	.00
17	8	18	9	31998.25	.00	.00
18	8	19	9	31997.41	.00	.00
10	10	11	11	31990.67	31990.85	.18
11	10	12	11	31989.95	31990.05	.10
12	10	13	11	31989.20	31989.30	.10
13	10	14	11	31988.45	.00	.00
14	10	15	11	31987.68	.00	.00
15	10	16	11	31986.89	.00	.00
16	10	17	11	31986.09	.00	.00
17	10	18	11	31985.27	.00	.00
18	10	19	11	31984.44	.00	.00
19	10	20	11	31983.59	.00	.00
20	10	21	11	31982.72	.00	.00
12	12	13	13	31974.77	31974.62	-.15
13	12	14	13	31974.01	31973.96	-.05
14	12	15	13	31973.24	31973.21	-.03
15	12	16	13	31972.46	31972.21	-.25
16	12	17	13	31971.66	31971.82	.16
17	12	18	13	31970.84	31970.96	.12
18	12	19	13	31970.01	31970.20	.19
19	12	20	13	31969.16	31969.50	.34
20	12	21	13	31968.30	31968.20	-.10
21	12	22	13	31967.43	.00	.00
22	12	23	13	31966.54	.00	.00
14	14	15	15	31957.37	31957.41	.04
15	14	16	15	31956.58	31956.68	.10
16	14	17	15	31955.78	31955.90	.12
17	14	18	15	31954.97	31954.86	-.11
18	14	19	15	31954.14	.00	.00
19	14	20	15	31953.30	.00	.00
20	14	21	15	31952.44	.00	.00
21	14	22	15	31951.56	.00	.00
22	14	23	15	31950.67	.00	.00
23	14	24	15	31949.77	.00	.00
24	14	25	15	31948.85	.00	.00
16	16	17	17	31938.47	.00	.00
17	16	18	17	31937.66	.00	.00
18	16	19	17	31936.83	.00	.00
19	16	20	17	31935.98	.00	.00
20	16	21	17	31935.13	.00	.00
21	16	22	17	31934.25	.00	.00
22	16	23	17	31933.37	.00	.00
23	16	24	17	31932.46	.00	.00
24	16	25	17	31931.55	.00	.00
25	16	26	17	31930.61	.00	.00
26	16	27	17	31929.67	.00	.00

Table 11. (Continued).

18	18	19	19	31918.07	.00	.00
19	18	20	19	31917.23	.00	.00
20	18	21	19	31916.37	.00	.00
21	18	22	19	31915.50	.00	.00
22	18	23	19	31914.62	.00	.00
23	18	24	19	31913.72	.00	.00
24	18	25	19	31912.80	.00	.00
25	18	26	19	31911.87	.00	.00
26	18	27	19	31910.92	.00	.00
27	18	28	19	31909.96	.00	.00
28	18	29	19	31908.99	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
2	2	1	1	32055.23	.00	.00
3	2	2	1	32055.67	.00	.00
4	2	3	1	32056.37	.00	.00
5	2	4	1	32056.53	.00	.00
6	2	5	1	32057.55	.00	.00
7	2	6	1	32057.26	.00	.00
8	2	7	1	32058.78	.00	.00
9	2	8	1	32057.87	.00	.00
10	2	9	1	32060.05	.00	.00
11	2	10	1	32058.37	.00	.00
12	2	11	1	32061.38	.00	.00
4	4	3	3	32060.60	32060.45	-.15
5	4	4	3	32061.10	32061.09	-.01
6	4	5	3	32061.58	32061.50	-.08
7	4	6	3	32062.05	32062.19	.14
8	4	7	3	32062.50	32062.50	.00
9	4	8	3	32062.93	32063.03	.10
10	4	9	3	32063.35	32063.31	-.04
11	4	10	3	32063.73	.00	.00
12	4	11	3	32064.13	.00	.00
13	4	12	3	32064.44	.00	.00
14	4	13	3	32064.84	.00	.00
6	6	5	5	32064.50	32064.60	.10
7	6	6	5	32064.97	32064.99	.02
8	6	7	5	32065.42	32065.60	.18
9	6	8	5	32065.86	32065.70	-.16
10	6	9	5	32066.28	32066.32	.04
11	6	10	5	32066.69	.00	.00
12	6	11	5	32067.08	.00	.00
13	6	12	5	32067.46	.00	.00
14	6	13	5	32067.81	.00	.00
15	6	14	5	32068.15	.00	.00
16	6	15	5	32068.48	.00	.00
8	8	7	7	32066.90	.00	.00
9	8	8	7	32067.34	.00	.00
10	8	9	7	32067.77	32067.65	-.12

Table 11. (Continued).

11	8	10	7	32068.18	32068.25	.07
12	8	11	7	32068.57	32068.50	-.07
13	8	12	7	32068.95	32069.00	.05
14	8	13	7	32069.32	32069.30	-.02
15	8	14	7	32069.66	.00	.00
16	8	15	7	32070.00	.00	.00
17	8	16	7	32070.31	.00	.00
18	8	17	7	32070.61	.00	.00
10	10	9	9	32067.81	32067.65	-.16
11	10	10	9	32068.22	32068.25	.03
12	10	11	9	32068.62	32068.50	-.12
13	10	12	9	32069.00	32069.00	.00
14	10	13	9	32069.36	.00	.00
15	10	14	9	32069.72	.00	.00
16	10	15	9	32070.05	.00	.00
17	10	16	9	32070.37	.00	.00
18	10	17	9	32070.68	.00	.00
19	10	18	9	32070.97	.00	.00
20	10	19	9	32071.24	.00	.00
12	12	11	11	32067.22	32067.15	-.07
13	12	12	11	32067.60	32067.65	.05
14	12	13	11	32067.97	.00	.00
15	12	14	11	32068.32	32068.25	-.07
16	12	15	11	32068.66	.00	.00
17	12	16	11	32068.98	.00	.00
18	12	17	11	32069.29	32069.30	.01
19	12	18	11	32069.58	.00	.00
20	12	19	11	32069.86	.00	.00
21	12	20	11	32070.12	.00	.00
22	12	21	11	32070.37	.00	.00
14	14	13	13	32065.13	32065.00	-.13
15	14	14	13	32065.48	32065.60	.12
16	14	15	13	32065.82	.00	.00
17	14	16	13	32066.15	32066.15	.00
18	14	17	13	32066.45	32066.32	-.13
19	14	18	13	32066.75	.00	.00
20	14	19	13	32067.03	.00	.00
21	14	20	13	32067.29	.00	.00
22	14	21	13	32067.54	.00	.00
23	14	22	13	32067.78	.00	.00
24	14	23	13	32067.99	.00	.00
16	16	15	15	32061.54	.00	.00
17	16	16	15	32061.87	.00	.00
18	16	17	15	32062.18	.00	.00
19	16	18	15	32062.47	.00	.00
20	16	19	15	32062.75	.00	.00
21	16	20	15	32063.02	.00	.00
22	16	21	15	32063.27	.00	.00
23	16	22	15	32063.51	.00	.00
24	16	23	15	32063.73	.00	.00
25	16	24	15	32063.93	.00	.00
26	16	25	15	32064.12	.00	.00

Table 11. (Continued).

18	18	17	17	32056.46	.00	.00
19	18	18	17	32056.76	.00	.00
20	18	19	17	32057.04	.00	.00
21	18	20	17	32057.30	.00	.00
22	18	21	17	32057.56	.00	.00
23	18	22	17	32057.79	.00	.00
24	18	23	17	32058.02	.00	.00
25	18	24	17	32058.22	.00	.00
26	18	25	17	32058.42	.00	.00
27	18	26	17	32058.59	.00	.00
28	18	27	17	32058.76	.00	.00
20	20	19	19	32049.88	.00	.00
21	20	20	19	32050.15	.00	.00
22	20	21	19	32050.40	.00	.00
23	20	22	19	32050.64	.00	.00
24	20	23	19	32050.86	.00	.00
25	20	24	19	32051.07	.00	.00
26	20	25	19	32051.27	.00	.00
27	20	26	19	32051.44	.00	.00
28	20	27	19	32051.61	.00	.00
29	20	28	19	32051.76	.00	.00
30	20	29	19	32051.89	.00	.00

Table 12. Observed and Calculated Transition Frequencies in cm^{-1} for the E Band of SO_2^{18}.

3 COLUMNS PROCESSED.
BAND ORIGIN AT 32714.806 CM-1.
B= .288239
A-C= 1.458635
DK= .000000000000
DJK= .000000000000
DJ= .000000000000
ROOT MEAN SQUARE DEVIATION= .1072 CM-1 FOR 55 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	3	3	4	4	32699.500	32699.628	-.128
2	4	3	5	4	32699.000	32699.086	-.086
3	5	3	6	4	32698.550	32698.552	-.002
4	6	3	7	4	32698.150	32698.023	.127
5	7	3	8	4	32697.520	32697.500	.020
6	8	3	9	4	32697.010	32696.982	.028
7	5	5	6	6	32689.280	32689.302	-.022
8	6	5	7	6	32688.950	32688.776	.174
9	8	5	9	6	32687.690	32687.742	-.052
10	9	5	10	6	32687.300	32687.234	.066
11	10	5	11	6	32686.900	32686.732	.167
12	11	5	12	6	32686.420	32686.236	.184
13	8	7	9	8	32677.140	32677.127	.013
14	9	7	10	8	32676.600	32676.621	-.021
15	10	7	11	8	32676.050	32676.122	-.072
16	11	7	12	8	32675.500	32675.629	-.129
17	12	7	13	8	32674.900	32675.142	-.242
18	13	7	14	8	32674.510	32674.662	-.152
19	14	7	15	8	32674.180	32674.187	-.007
20	9	9	10	10	32664.840	32664.638	.202
21	10	9	11	10	32664.310	32664.140	.170
22	11	9	12	10	32663.680	32663.648	.031
23	12	9	13	10	32663.190	32663.164	.026
24	13	9	14	10	32662.450	32662.685	-.235
25	14	9	15	10	32662.230	32662.213	.017
26	15	9	16	10	32661.810	32661.748	.063
27	16	9	17	10	32661.420	32661.288	.132
28	11	11	12	12	32650.300	32650.299	.001
29	12	11	13	12	32649.900	32649.815	.085
30	13	13	14	14	32634.600	32634.622	-.022
31	14	13	15	14	32634.120	32634.152	-.032
32	15	13	16	14	32633.680	32633.689	-.010
33	16	13	17	14	32633.250	32633.233	.017
34	17	13	18	14	32632.900	32632.784	.116
35	18	13	19	14	32632.420	32632.341	.079
36	15	15	16	16	32617.400	32617.607	-.207

Table 12. (Continued).

37	16	15	17	16	32617.090	32617.152	-.062
38	17	15	18	16	32616.760	32616.703	.057
39	3	3	2	2	32723.020	32723.166	-.146
40	4	3	3	2	32723.780	32723.766	.014
41	5	3	4	2	32724.300	32724.360	-.060
42	6	3	5	2	32725.180	32724.988	.192
43	7	3	6	2	32725.600	32725.554	.046
44	8	3	7	2	32726.200	32726.248	-.048
45	9	3	8	2	32726.640	32726.722	-.082
46	10	3	9	2	32727.350	32727.552	-.202
47	11	3	10	2	32727.800	32727.830	-.030
48	13	3	12	2	32728.900	32728.853	.047
49	5	5	4	4	32728.200	32728.154	.046
50	6	5	5	4	32728.900	32728.766	.134
51	7	5	6	4	32729.430	32729.384	.046
52	8	5	7	4	32729.950	32730.009	-.059
53	9	5	8	4	32730.600	32730.638	-.038
54	10	5	9	4	32731.250	32731.274	-.024
55	11	5	10	4	32731.790	32731.914	-.124

Table 12. (Continued).

* * * * * * * * P BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	2	2	32708.61	.00	.00
2	1	3	2	32708.06	.00	.00
3	1	4	2	32707.50	.00	.00
4	1	5	2	32706.98	.00	.00
5	1	6	2	32706.39	.00	.00
6	1	7	2	32705.93	.00	.00
7	1	8	2	32705.25	.00	.00
8	1	9	2	32704.93	.00	.00
9	1	10	2	32704.05	.00	.00
10	1	11	2	32703.98	.00	.00
11	1	12	2	32702.77	.00	.00
3	3	4	4	32699.63	32699.50	-.13
4	3	5	4	32699.09	32699.00	-.09
5	3	6	4	32698.55	32698.55	-.00
6	3	7	4	32698.02	32698.15	.13
7	3	8	4	32697.50	32697.52	.02
8	3	9	4	32696.98	32697.01	.03
9	3	10	4	32696.47	.00	.00
10	3	11	4	32695.96	.00	.00
11	3	12	4	32695.45	.00	.00
12	3	13	4	32694.95	.00	.00
13	3	14	4	32694.45	.00	.00
5	5	6	6	32689.30	32689.28	-.02
6	5	7	6	32688.78	32688.95	.17
7	5	8	6	32688.26	.00	.00
8	5	9	6	32687.74	32687.69	-.05
9	5	10	6	32687.23	32687.30	.07
10	5	11	6	32686.73	32686.90	.17
11	5	12	6	32686.24	32686.42	.18
12	5	13	6	32685.75	.00	.00
13	5	14	6	32685.26	.00	.00
14	5	15	6	32684.78	.00	.00
15	5	16	6	32684.30	.00	.00
7	7	8	8	32677.64	.00	.00
8	7	9	8	32677.13	32677.14	.01
9	7	10	8	32676.62	32676.60	-.02
10	7	11	8	32676.12	32676.05	-.07
11	7	12	8	32675.63	32675.50	-.13
12	7	13	8	32675.14	32674.90	-.24
13	7	14	8	32674.66	32674.51	-.15
14	7	15	8	32674.19	32674.18	-.01
15	7	16	8	32673.72	.00	.00
16	7	17	8	32673.25	.00	.00
17	7	18	8	32672.80	.00	.00
9	9	10	10	32664.64	32664.84	.20
10	9	11	10	32664.14	32664.31	.17
11	9	12	10	32663.65	32663.68	.03
12	9	13	10	32663.16	32663.19	.03
13	9	14	10	32662.69	32662.45	-.24
14	9	15	10	32662.21	32662.23	.02
15	9	16	10	32661.75	32661.81	.06
16	9	17	10	32661.29	32661.42	.13
17	9	18	10	32660.83	.00	.00

Table 12. (Continued).

18	9	19	10	32660.39	.00	.00
19	9	20	10	32659.94	.00	.00
11	11	12	12	32650.30	32650.30	.00
12	11	13	12	32649.82	32649.90	.08
13	11	14	12	32649.34	.00	.00
14	11	15	12	32648.87	.00	.00
15	11	16	12	32648.40	.00	.00
16	11	17	12	32647.95	.00	.00
17	11	18	12	32647.50	.00	.00
18	11	19	12	32647.05	.00	.00
19	11	20	12	32646.61	.00	.00
20	11	21	12	32646.18	.00	.00
21	11	22	12	32645.75	.00	.00
13	13	14	14	32634.62	32634.60	-.02
14	13	15	14	32634.15	32634.12	-.03
15	13	16	14	32633.69	32633.68	-.01
16	13	17	14	32633.23	32633.25	.02
17	13	18	14	32632.78	32632.90	.12
18	13	19	14	32632.34	32632.42	.08
19	13	20	14	32631.90	.00	.00
20	13	21	14	32631.47	.00	.00
21	13	22	14	32631.05	.00	.00
22	13	23	14	32630.63	.00	.00
23	13	24	14	32630.22	.00	.00
15	15	16	16	32617.61	32617.40	-.21
16	15	17	16	32617.15	32617.09	-.06
17	15	18	16	32616.70	32616.76	.06
18	15	19	16	32616.26	.00	.00
19	15	20	16	32615.83	.00	.00
20	15	21	16	32615.40	.00	.00
21	15	22	16	32614.98	.00	.00
22	15	23	16	32614.56	.00	.00
23	15	24	16	32614.15	.00	.00
24	15	25	16	32613.75	.00	.00
25	15	26	16	32613.35	.00	.00
17	17	18	18	32599.25	.00	.00
18	17	19	18	32598.81	.00	.00
19	17	20	18	32598.38	.00	.00
20	17	21	18	32597.95	.00	.00
21	17	22	18	32597.53	.00	.00
22	17	23	18	32597.12	.00	.00
23	17	24	18	32596.71	.00	.00
24	17	25	18	32596.31	.00	.00
25	17	26	18	32595.91	.00	.00
26	17	27	18	32595.52	.00	.00
27	17	28	18	32595.14	.00	.00
19	19	20	20	32579.56	.00	.00
20	19	21	20	32579.14	.00	.00
21	19	22	20	32578.72	.00	.00
22	19	23	20	32578.30	.00	.00
23	19	24	20	32577.90	.00	.00
24	19	25	20	32577.50	.00	.00
25	19	26	20	32577.10	.00	.00
26	19	27	20	32576.72	.00	.00
27	19	28	20	32576.34	.00	.00

Table 12. (Continued).

28	19	29	20	32575.96	.00	.00
29	19	30	20	32575.60	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	0	0	32716.84	.00	.00
2	1	1	0	32717.99	.00	.00
3	1	2	0	32718.02	.00	.00
4	1	3	0	32722.03	.00	.00
5	1	4	0	32719.23	.00	.00
6	1	5	0	32728.37	.00	.00
7	1	6	0	32720.51	.00	.00
8	1	7	0	32737.02	.00	.00
9	1	8	0	32721.89	.00	.00
10	1	9	0	32747.97	.00	.00
11	1	10	0	32723.41	.00	.00
3	3	2	2	32723.17	32723.02	-.15
4	3	3	2	32723.77	32723.78	.01
5	3	4	2	32724.36	32724.30	-.06
6	3	5	2	32724.99	32725.18	.19
7	3	6	2	32725.55	32725.60	.05
8	3	7	2	32726.25	32726.20	-.05
9	3	8	2	32726.72	32726.64	-.08
10	3	9	2	32727.55	32727.35	-.20
11	3	10	2	32727.83	32727.80	-.03
12	3	11	2	32728.91	.00	.00
13	3	12	2	32728.85	32728.90	.05
5	5	4	4	32728.15	32728.20	.05
6	5	5	4	32728.77	32728.90	.13
7	5	6	4	32729.38	32729.43	.05
8	5	7	4	32730.01	32729.95	-.06
9	5	8	4	32730.64	32730.60	-.04
10	5	9	4	32731.27	32731.25	-.02
11	5	10	4	32731.91	32731.79	-.12
12	5	11	4	32732.56	.00	.00
13	5	12	4	32733.20	.00	.00
14	5	13	4	32733.86	.00	.00
15	5	14	4	32734.51	.00	.00
7	7	6	6	32731.80	.00	.00
8	7	7	6	32732.43	.00	.00
9	7	8	6	32733.06	.00	.00
10	7	9	6	32733.70	.00	.00
11	7	10	6	32734.35	.00	.00
12	7	11	6	32735.00	.00	.00
13	7	12	6	32735.66	.00	.00
14	7	13	6	32736.32	.00	.00
15	7	14	6	32736.99	.00	.00
16	7	15	6	32737.66	.00	.00
17	7	16	6	32738.33	.00	.00
9	9	8	8	32734.12	.00	.00
10	9	9	8	32734.76	.00	.00
11	9	10	8	32735.40	.00	.00
12	9	11	8	32736.06	.00	.00
13	9	12	8	32736.72	.00	.00
14	9	13	8	32737.38	.00	.00

Table 12. (Continued).

15	9	14	8	32738.06	.00	.00
16	9	15	8	32738.73	.00	.00
17	9	16	8	32739.42	.00	.00
18	9	17	8	32740.11	.00	.00
19	9	18	8	32740.80	.00	.00
11	11	10	10	32735.09	.00	.00
12	11	11	10	32735.74	.00	.00
13	11	12	10	32736.41	.00	.00
14	11	13	10	32737.07	.00	.00
15	11	14	10	32737.75	.00	.00
16	11	15	10	32738.43	.00	.00
17	11	16	10	32739.12	.00	.00
18	11	17	10	32739.81	.00	.00
19	11	18	10	32740.51	.00	.00
20	11	19	10	32741.21	.00	.00
21	11	20	10	32741.93	.00	.00
13	13	12	12	32734.73	.00	.00
14	13	13	12	32735.39	.00	.00
15	13	14	12	32736.07	.00	.00
16	13	15	12	32736.75	.00	.00
17	13	16	12	32737.44	.00	.00
18	13	17	12	32738.14	.00	.00
19	13	18	12	32738.84	.00	.00
20	13	19	12	32739.55	.00	.00
21	13	20	12	32740.26	.00	.00
22	13	21	12	32740.98	.00	.00
23	13	22	12	32741.71	.00	.00
15	15	14	14	32733.02	.00	.00
16	15	15	14	32733.71	.00	.00
17	15	16	14	32734.40	.00	.00
18	15	17	14	32735.09	.00	.00
19	15	18	14	32735.80	.00	.00
20	15	19	14	32736.51	.00	.00
21	15	20	14	32737.22	.00	.00
22	15	21	14	32737.95	.00	.00
23	15	22	14	32738.68	.00	.00
24	15	23	14	32739.41	.00	.00
25	15	24	14	32740.15	.00	.00
17	17	16	16	32729.98	.00	.00
18	17	17	16	32730.68	.00	.00
19	17	18	16	32731.39	.00	.00
20	17	19	16	32732.10	.00	.00
21	17	20	16	32732.81	.00	.00
22	17	21	16	32733.54	.00	.00
23	17	22	16	32734.27	.00	.00
24	17	23	16	32735.01	.00	.00
25	17	24	16	32735.75	.00	.00
26	17	25	16	32736.50	.00	.00
27	17	26	16	32737.26	.00	.00
19	19	18	18	32725.61	.00	.00
20	19	19	18	32726.32	.00	.00
21	19	20	18	32727.04	.00	.00
22	19	21	18	32727.76	.00	.00
23	19	22	18	32728.49	.00	.00
24	19	23	18	32729.23	.00	.00

Table 12. (Continued).

25	19	24	18	32729.98	.00	.00
26	19	25	18	32730.73	.00	.00
27	19	26	18	32731.49	.00	.00
28	19	27	18	32732.25	.00	.00
29	19	28	18	32733.02	.00	.00

Table 13. Observed and Calculated Transition Frequencies in cm^{-1} for the F Band of SO_2^{18}.

BAND ORIGIN AT 32936.253 CM-1.
B= .289739
A-C= 1.464067
DK= .0000000000000
DJK= .0000000000000
DJ= .0000000000000
ROOT MEAN SQUARE DEVIATION= .1032 CM-1 FOR 91 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	2	2	3	3	32925.620	32925.766	-.146
2	3	2	4	3	32925.250	32925.227	.023
3	4	2	5	3	32924.840	32924.656	.184
4	5	2	6	3	32924.060	32924.174	-.114
5	6	2	7	3	32923.680	32923.662	.018
6	4	4	5	5	32916.300	32916.196	.104
7	6	4	7	5	32915.100	32915.167	-.067
8	7	4	8	5	32914.700	32914.667	.033
9	7	6	8	7	32904.880	32904.845	.035
10	8	6	9	7	32904.400	32904.356	.044
11	9	6	10	7	32903.910	32903.876	.034
12	10	6	11	7	32903.200	32903.406	-.206
13	12	6	13	7	32902.600	32902.493	.107
14	13	6	14	7	32902.110	32902.049	.061
15	14	6	15	7	32901.600	32901.614	-.014
16	15	6	16	7	32901.300	32901.187	.113
17	8	8	9	9	32893.130	32893.208	-.078
18	9	8	10	9	32892.700	32892.730	-.030
19	10	8	11	9	32892.300	32892.261	.039
20	10	10	11	11	32879.700	32879.791	-.090
21	11	10	12	11	32879.390	32879.333	.058
22	12	10	13	11	32878.900	32878.884	.016
23	13	10	14	11	32878.450	32878.445	.005
24	14	10	15	11	32878.120	32878.016	.104
25	15	10	16	11	32877.690	32877.597	.093
26	16	10	17	11	32877.310	32877.186	.124
27	17	10	18	11	32876.990	32876.785	.205
28	18	10	19	11	32876.640	32876.393	.247
29	19	10	20	11	32876.100	32876.010	.090
30	12	12	13	13	32865.190	32865.090	.100
31	13	12	14	13	32864.740	32864.653	.087
32	15	12	16	13	32863.720	32863.806	-.086
33	16	12	17	13	32863.430	32863.397	.033
34	17	12	18	13	32863.000	32862.999	.001
35	18	12	19	13	32862.400	32862.608	-.208
36	19	12	20	13	32862.180	32862.228	-.048
37	20	12	21	13	32861.780	32861.857	-.077
38	21	12	22	13	32861.260	32861.495	-.235
39	14	14	15	15	32849.060	32849.108	-.048
40	15	14	16	15	32848.600	32848.690	-.090
41	18	14	19	15	32847.500	32847.496	.004
42	19	14	20	15	32847.200	32847.118	.083
43	20	14	21	15	32846.850	32846.749	.102
44	23	14	24	15	32845.610	32845.697	-.087
45	6	6	7	7	32905.300	32905.343	-.043
46	2	2	1	1	32941.640	32941.670	-.030
47	3	2	2	1	32942.200	32942.185	.016
48	4	2	3	1	32943.210	32942.988	.222
49	6	2	5	1	32944.400	32944.438	-.039
50	4	4	3	3	32947.400	32947.391	.009
51	5	4	4	3	32947.980	32948.011	-.031

Table 13. (Continued).

52	6	4	5	3	32948.700	32948.639	.061
53	7	4	6	3	32949.150	32949.276	-.126
54	8	4	7	3	32949.950	32949.923	.027
55	9	4	8	3	32950.600	32950.573	.027
56	10	4	9	3	32951.250	32951.239	.011
57	11	4	10	3	32951.800	32951.890	-.090
58	12	4	11	3	32952.650	32952.583	.067
59	13	4	12	3	32953.200	32953.215	-.015
60	14	4	13	3	32954.000	32953.955	.045
61	6	6	5	5	32951.800	32951.852	-.052
62	7	6	6	5	32952.450	32952.491	-.041
63	8	6	7	5	32953.100	32953.141	-.041
64	9	6	8	5	32953.650	32953.800	-.150
65	12	6	11	5	32955.900	32955.829	.071
66	13	6	12	5	32956.450	32956.521	-.071
67	8	8	7	7	32955.000	32955.029	-.029
68	9	8	8	7	32955.710	32955.689	.021
69	10	8	9	7	32956.230	32956.359	-.129
70	11	8	10	7	32957.000	32957.039	-.039
71	12	8	11	7	32957.710	32957.728	-.018
72	13	8	12	7	32958.290	32958.426	-.136
73	14	8	13	7	32959.200	32959.132	.068
74	15	8	14	7	32959.900	32959.848	.052
75	10	10	9	9	32956.900	32956.925	-.025
76	11	10	10	9	32957.470	32957.605	-.135
77	12	10	11	9	32958.290	32958.295	-.005
78	14	10	13	9	32959.720	32959.705	.016
79	12	12	11	11	32957.710	32957.538	.172
80	13	12	12	11	32958.290	32958.238	.052
81	14	12	13	11	32958.900	32958.949	-.049
82	15	12	14	11	32959.720	32959.669	.051
83	16	12	15	11	32960.320	32960.399	-.079
84	17	12	16	11	32961.100	32961.138	-.038
85	18	12	17	11	32961.900	32961.887	.013
86	19	12	18	11	32962.350	32962.645	-.295
87	20	12	19	11	32963.550	32963.412	.138
88	21	12	20	11	32963.900	32964.187	-.288
89	18	14	17	13	32959.900	32959.811	.089
90	20	14	19	13	32961.510	32961.340	.170
91	23	14	22	13	32963.800	32963.703	.097

Table 13. (Continued).

* * * * * * * * P BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
0	0	1	1	32934.08	.00	.00
1	0	2	1	32933.43	.0	.0[illegible]
2	0	3	1	32933.08	.0[illegible]	.0[illegible]
3	0	4	1	32932.20	.00	.00
4	0	5	1	32932.21	.00	.00
5	0	6	1	32930.93	.00	.00
6	0	7	1	32931.48	.00	.00
7	0	8	1	32929.64	.00	.00
8	0	9	1	32930.90	.00	.00
9	0	10	1	32928.33	.00	.00
10	0	11	1	32930.48	.00	.00
2	2	3	3	32925.77	32925.62	-.15
3	2	4	3	32925.23	32925.25	.02
4	2	5	3	32924.70	32924.88	.18
5	2	6	3	32924.17	32924.06	-.11
6	2	7	3	32923.6[illegible]	32923.68	.02
7	2	8	3	32923.15	.0	.0[illegible]
8	2	9	3	32922.66	.00	.00
9	2	10	3	32922.15	.00	.00
10	2	11	3	32921.69	.00	.00
11	2	12	3	32921.16	.00	.00
12	2	13	3	32920.74	.00	.00
4	4	5	5	32916.20	32916.30	.10
5	4	6	5	32915.68	.00	.00
6	4	7	5	32915.17	32915.10	-.07
7	4	8	5	32914.67	32914.70	.03
8	4	9	5	32914.18	.00	.00
9	4	10	5	32913.69	.00	.00
10	4	11	5	32913.22	.00	.00
11	4	12	5	32912.75	.00	.00
12	4	13	5	32912.29	.00	.00
13	4	14	5	32911.84	.00	.00
14	4	15	5	32911.40	.00	.00
6	6	7	7	32905.34	32905.30	-.04
7	6	8	7	32904.84	32904.88	.04
8	6	9	7	32904.36	32904.40	.04
9	6	10	7	32903.88	32903.91	.03
10	6	11	7	32903.41	32903.20	-.21
11	6	12	7	32902.94	.00	.00
12	6	13	7	32902.49	32902.60	.11
13	6	14	7	32902.05	32902.11	.06
14	6	15	7	32901.61	32901.60	-.01
15	6	16	7	32901.19	32901.30	.11
16	6	17	7	32900.77	.00	.00
8	8	9	9	32893.21	32893.13	-.08
9	8	10	9	32892.73	32892.70	-.03
10	8	11	9	32892.26	32892.30	.04

Table 13. (Continued).

11	8	12	9	32891.80	.00	.00
12	8	13	9	32891.35	.00	.00
13	8	14	9	32890.91	.00	.00
14	8	15	9	32890.48	.00	.00
15	8	16	9	32890.06	.00	.00
16	8	17	9	32889.65	.00	.00
17	8	18	9	32889.24	.00	.00
18	8	19	9	32888.85	.00	.00
10	10	11	11	32879.79	32879.70	-.09
11	10	12	11	32879.33	32879.39	.06
12	10	13	11	32878.88	32878.90	.02
13	10	14	11	32878.45	32878.45	.00
14	10	15	11	32878.02	32878.12	.10
15	10	16	11	32877.60	32877.69	.09
16	10	17	11	32877.19	32877.31	.12
17	10	18	11	32876.79	32876.99	.21
18	10	19	11	32876.39	32876.64	.25
19	10	20	11	32876.01	32876.10	.09
20	10	21	11	32875.64	.00	.00
12	12	13	13	32865.09	32865.19	.10
13	12	14	13	32864.65	32864.74	.09
14	12	15	13	32864.22	.00	.00
15	12	16	13	32863.81	32863.72	-.09
16	12	17	13	32863.40	32863.43	.03
17	12	18	13	32863.00	32863.00	.00
18	12	19	13	32862.61	32862.40	-.21
19	12	20	13	32862.23	32862.18	-.05
20	12	21	13	32861.86	32861.78	-.08
21	12	22	13	32861.50	32861.26	-.24
22	12	23	13	32861.14	.00	.00
14	14	15	15	32849.11	32849.06	-.05
15	14	16	15	32848.69	32848.60	-.09
16	14	17	15	32848.28	.00	.00
17	14	18	15	32847.88	.00	.00
18	14	19	15	32847.50	32847.50	.00
19	14	20	15	32847.12	32847.20	.08
20	14	21	15	32846.75	32846.85	.10
21	14	22	15	32846.39	.00	.00
22	14	23	15	32846.04	.00	.00
23	14	24	15	32845.70	32845.61	-.09
24	14	25	15	32845.36	.00	.00
16	16	17	17	32831.84	.00	.00
17	16	18	17	32831.45	.00	.00
18	16	19	17	32831.06	.00	.00
19	16	20	17	32830.68	.00	.00
20	16	21	17	32830.31	.00	.00
21	16	22	17	32829.95	.00	.00
22	16	23	17	32829.61	.00	.00
23	16	24	17	32829.27	.00	.00
24	16	25	17	32828.94	.00	.00
25	16	26	17	32828.62	.00	.00
26	16	27	17	32828.30	.00	.00

Table 13. (Continued).

18	18	19	19	32813.29	.00	.00
19	18	20	19	32812.92	.00	.00
20	18	21	19	32812.55	.00	.00
21	18	22	19	32812.19	.00	.00
22	18	23	19	32811.85	.00	.00
23	18	24	19	32811.51	.00	.0
24	18	25	19	32811.18	.00	.00
25	18	26	19	32810.86	.00	.00
26	18	27	19	32810.55	.00	.00
27	18	28	19	32810.25	.00	.00
28	18	29	19	32809.96	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
2	2	1	1	32941.67	32941.64	-.03
3	2	2	1	32942.18	32942.20	.02
4	2	3	1	32942.99	32943.21	.22
5	2	4	1	32943.27	.00	.00
6	2	5	1	32944.44	32944.40	-.04
7	2	6	1	32944.32	.00	.0
8	2	7	1	32946.03	.00	.00
9	2	8	1	32945.34	.00	.00
10	2	9	1	32947.76	.00	.00
11	2	10	1	32946.36	.00	.00
12	2	11	1	32949.66	.00	.00
4	4	3	3	32947.39	32947.40	.01
5	4	4	3	32948.01	32947.98	-.03
6	4	5	3	32948.64	32948.70	.06
7	4	6	3	32949.28	32949.15	-.13
8	4	7	3	32949.92	32949.95	.03
9	4	8	3	32950.57	32950.60	.03
10	4	9	3	32951.24	32951.25	.01
11	4	10	3	32951.89	32951.80	-.09
12	4	11	3	32952.58	32952.65	.07
13	4	12	3	32953.21	32953.20	-.01
14	4	13	3	32953.95	32954.00	.05
6	6	5	5	32951.85	32951.80	-.05
7	6	6	5	32952.49	32952.45	-.04
8	6	7	5	32953.14	32953.10	-.04
9	6	8	5	32953.80	32953.65	-.15
10	6	9	5	32954.47	.00	.00
11	6	10	5	32955.14	.00	.00
12	6	11	5	32955.83	32955.90	.07
13	6	12	5	32956.52	32956.45	-.07
14	6	13	5	32957.22	.00	.00
15	6	14	5	32957.93	.00	.00
16	6	15	5	32958.64	.00	.00
8	8	7	7	32955.03	32955.00	-.03
9	8	8	7	32955.69	32955.71	.02
10	8	9	7	32956.36	32956.23	-.13

Table 13. (Continued).

11	8	10	7	32957.04	32957.00	-.04
12	8	11	7	32957.73	32957.71	-.02
13	8	12	7	32958.43	32958.29	-.14
14	8	13	7	32959.13	32959.20	.07
15	8	14	7	32959.85	32959.90	.05
16	8	15	7	32960.57	.00	.00
17	8	16	7	32961.30	.00	.00
18	8	17	7	32962.04	.00	.00
10	10	9	9	32956.92	32956.90	-.02
11	10	10	9	32957.60	32957.47	-.13
12	10	11	9	32958.30	32958.29	-.01
13	10	12	9	32959.00	.00	.00
14	10	13	9	32959.70	32959.72	.02
15	10	14	9	32960.42	.00	.00
16	10	15	9	32961.15	.00	.00
17	10	16	9	32961.89	.00	.00
18	10	17	9	32962.63	.00	.00
19	10	18	9	32963.39	.00	.00
20	10	19	9	32964.15	.00	.00
12	12	11	11	32957.54	32957.71	.17
13	12	12	11	32958.24	32958.29	.05
14	12	13	11	32958.95	32958.90	-.05
15	12	14	11	32959.67	32959.72	.05
16	12	15	11	32960.40	32960.32	-.08
17	12	16	11	32961.14	32961.10	-.04
18	12	17	11	32961.89	32961.90	.01
19	12	18	11	32962.65	32962.35	-.29
20	12	19	11	32963.41	32963.55	.14
21	12	20	11	32964.19	32963.90	-.29
22	12	21	11	32964.97	.00	.00
14	14	13	13	32956.87	.00	.00
15	14	14	13	32957.59	.00	.00
16	14	15	13	32958.32	.00	.00
17	14	16	13	32959.06	.00	.00
18	14	17	13	32959.81	32959.90	.09
19	14	18	13	32960.57	.00	.00
20	14	19	13	32961.34	32961.51	.17
21	14	20	13	32962.12	.00	.00
22	14	21	13	32962.91	.00	.00
23	14	22	13	32963.70	32963.80	.10
24	14	23	13	32964.51	.00	.00
16	16	15	15	32954.92	.00	.00
17	16	16	15	32955.66	.00	.00
18	16	17	15	32956.41	.00	.00
19	16	18	15	32957.17	.00	.00
20	16	19	15	32957.94	.00	.00
21	16	20	15	32958.72	.00	.00
22	16	21	15	32959.51	.00	.00
23	16	22	15	32960.31	.00	.00
24	16	23	15	32961.12	.00	.00
25	16	24	15	32961.94	.00	.00
26	16	25	15	32962.76	.00	.00

Table 13. (Continued).

18	18	17	17	32951.68	.00	.00
19	18	18	17	32952.44	.00	.00
20	18	19	17	32953.21	.00	.00
21	18	20	17	32954.00	.00	.00
22	18	21	17	32954.79	.00	.00
23	18	22	17	32955.59	.00	.00
24	18	23	17	32956.40	.00	.00
25	18	24	17	32957.22	.00	.00
26	18	25	17	32958.05	.00	.00
27	18	26	17	32958.88	.00	.00
28	18	27	17	32959.73	.00	.00

20	20	19	19	32947.16	.00	.00
21	20	20	19	32947.95	.00	.00
22	20	21	19	32948.74	.00	.00
23	20	22	19	32949.54	.00	.00
24	20	23	19	32950.35	.00	.00
25	20	24	19	32951.17	.00	.00
26	20	25	19	32952.00	.00	.00
27	20	26	19	32952.84	.00	.00
28	20	27	19	32953.69	.00	.00
29	20	28	19	32954.55	.00	.00
30	20	29	19	32955.42	.00	.00

Table 14. Observed and Calculated Transition Frequencies in cm^{-1} for the G Band of SO_2^{18}.

BAND ORIGIN AT 33153.359 CM-1.
B= .288921
A-C= 1.461962
DK= .000000000000
DJK= .000000000000
DJ= .000000000000
ROOT MEAN SQUARE DEVIATION= .1052 CM-1 FOR 77 LINES.

INDEX	J'	K'	J"	K"	FREQ OBS	FREQ CALC	DIFFERENCE
1	3	3	4	4	33138.280	33138.219	.061
2	4	3	5	4	33137.810	33137.683	.127
3	5	3	6	4	33136.970	33137.155	-.185
4	6	3	7	4	33136.570	33136.635	-.065
5	8	3	9	4	33135.750	33135.615	.135
6	11	3	12	4	33134.220	33134.128	.092
7	5	5	6	6	33128.090	33127.959	.130
8	6	5	7	6	33127.310	33127.440	-.130
9	9	5	10	6	33125.800	33125.932	-.132
10	10	5	11	6	33125.500	33125.444	.056
11	11	5	12	6	33125.060	33124.963	.097
12	7	7	8	8	33116.400	33116.394	.006
13	8	7	9	8	33115.820	33115.892	-.072
14	9	7	10	8	33115.490	33115.398	.092
15	10	7	11	8	33115.070	33114.913	.157
16	11	7	12	8	33114.580	33114.435	.145
17	12	7	13	8	33113.960	33113.965	-.005
18	13	7	14	8	33113.430	33113.502	-.072
19	15	7	16	8	33112.520	33112.598	-.078
20	9	9	10	10	33103.500	33103.522	-.022
21	11	9	12	10	33102.550	33102.561	-.011
22	13	9	14	10	33101.610	33101.632	-.022
23	14	9	15	10	33101.210	33101.179	.031
24	15	9	16	10	33100.850	33100.734	.116
25	16	9	17	10	33100.450	33100.296	.154
26	17	9	18	10	33100.000	33099.866	.134
27	11	11	12	12	33089.300	33089.345	-.045
28	12	11	13	12	33088.850	33088.877	-.027
29	13	11	14	12	33088.500	33088.418	.082
30	14	11	15	12	33088.000	33087.966	.034
31	15	11	16	12	33087.410	33087.523	-.113
32	16	11	17	12	33087.000	33087.087	-.087
33	17	11	18	12	33086.600	33086.660	-.060
34	18	11	19	12	33086.290	33086.239	.051
35	19	11	20	12	33085.950	33085.827	.124
36	20	11	21	12	33085.400	33085.421	-.021
37	21	11	22	12	33084.940	33085.023	-.083
38	4	3	3	2	33162.410	33162.362	.048
39	5	3	4	2	33162.856	33162.963	-.107
40	8	3	7	2	33164.850	33164.880	-.030
41	9	3	8	2	33165.100	33165.366	-.266
42	10	3	9	2	33166.231	33166.210	.021
43	12	3	11	2	33167.620	33167.601	.020
44	13	3	12	2	33167.500	33167.561	-.061
45	5	5	4	4	33166.800	33166.811	-.011
46	6	5	5	4	33167.480	33167.431	.049
47	7	5	6	4	33168.050	33168.059	-.009

Table 14. (Continued).

48	8	5	7	4	33168.710	33168.694	.016
49	9	5	8	4	33169.321	33169.336	-.015
50	13	5	12	4	33172.000	33171.965	.035
51	14	5	13	4	33172.670	33172.637	.033
52	10	7	9	6	33172.411	33172.493	-.082
53	12	7	11	6	33173.750	33173.821	-.071
54	13	7	12	6	33174.400	33174.496	-.096
55	9	9	8	8	33173.100	33173.000	.100
56	10	9	9	8	33173.550	33173.654	-.104
57	11	9	10	8	33174.412	33174.316	.096
58	13	9	12	8	33175.900	33175.664	.236
59	15	9	14	8	33177.220	33177.042	.178
60	16	9	15	8	33177.580	33177.742	-.162
61	17	9	16	8	33178.500	33178.449	.051
62	18	9	17	8	33179.070	33179.164	-.094
63	11	11	10	10	33174.000	33174.135	-.135
64	13	11	12	10	33175.300	33175.486	-.186
65	14	11	13	10	33176.100	33176.173	-.073
66	15	11	14	10	33176.800	33176.868	-.068
67	16	11	15	10	33177.580	33177.571	.009
68	17	11	16	10	33178.290	33178.281	.009
69	18	11	17	10	33179.060	33178.999	.061
70	20	11	19	10	33180.500	33180.457	.043
71	21	11	20	10	33181.070	33181.197	-.127
72	14	7	15	8	33112.940	33113.046	-.106
73	6	3	5	2	33163.400	33163.600	-.200
74	7	3	6	2	33164.200	33164.176	.024
75	11	3	10	2	33166.500	33166.503	-.003
76	7	7	6	6	33170.650	33170.558	.092
77	12	9	11	8	33175.300	33174.986	.314

Table 14. (Continued).

* * * * * * * * P BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	2	2	33147.17	.00	.00
2	1	3	2	33146.62	.00	.00
3	1	4	2	33146.07	.00	.00
4	1	5	2	33145.55	.00	.00
5	1	6	2	33144.97	.00	.00
6	1	7	2	33144.52	.00	.00
7	1	8	2	33143.85	.00	.00
8	1	9	2	33143.54	.00	.00
9	1	10	2	33142.67	.00	.00
10	1	11	2	33142.61	.00	.00
11	1	12	2	33141.42	.00	.00
3	3	4	4	33138.22	33138.28	.06
4	3	5	4	33137.68	33137.81	.13
5	3	6	4	33137.16	33136.97	-.19
6	3	7	4	33136.63	33136.57	-.06
7	3	8	4	33136.12	.00	.00
8	3	9	4	33135.61	33135.75	.14
9	3	10	4	33135.11	.00	.00
10	3	11	4	33134.62	.00	.00
11	3	12	4	33134.13	33134.22	.09
12	3	13	4	33133.64	.00	.00
13	3	14	4	33133.16	.00	.00
5	5	6	6	33127.96	33128.09	.13
6	5	7	6	33127.44	33127.31	-.13
7	5	8	6	33126.93	.00	.00
8	5	9	6	33126.43	.00	.00
9	5	10	6	33125.93	33125.80	-.13
10	5	11	6	33125.44	33125.50	.06
11	5	12	6	33124.96	33125.06	.10
12	5	13	6	33124.49	.00	.00
13	5	14	6	33124.02	.00	.00
14	5	15	6	33123.56	.00	.00
15	5	16	6	33123.10	.00	.00
7	7	8	8	33116.39	33116.40	.01
8	7	9	8	33115.89	33115.82	-.07
9	7	10	8	33115.40	33115.49	.09
10	7	11	8	33114.91	33115.07	.16
11	7	12	8	33114.44	33114.58	.15
12	7	13	8	33113.96	33113.96	-.00
13	7	14	8	33113.50	33113.43	-.07
14	7	15	8	33113.05	33112.94	-.11
15	7	16	8	33112.60	33112.52	-.08
16	7	17	8	33112.16	.00	.00
17	7	18	8	33111.72	.00	.00
9	9	10	10	33103.52	33103.50	-.02
10	9	11	10	33103.04	.00	.00
11	9	12	10	33102.56	33102.55	-.01
12	9	13	10	33102.09	.00	.00
13	9	14	10	33101.63	33101.61	-.02
14	9	15	10	33101.18	33101.21	.03
15	9	16	10	33100.73	33100.85	.12
16	9	17	10	33100.30	33100.45	.15

Table 14. (Continued).

17	9	18	10	33099.87	33100.00	.13
18	9	19	10	33099.44	.00	.00
19	9	20	10	33099.03	.00	.00
11	11	12	12	33089.34	33089.30	-.04
12	11	13	12	33088.88	33088.85	-.03
13	11	14	12	33088.42	33088.50	.08
14	11	15	12	33087.97	33088.00	.03
15	11	16	12	33087.52	33087.41	-.11
16	11	17	12	33087.09	33087.00	-.09
17	11	18	12	33086.66	33086.60	-.06
18	11	19	12	33086.24	33086.29	.05
19	11	20	12	33085.83	33085.95	.12
20	11	21	12	33085.42	33085.40	-.02
21	11	22	12	33085.02	33084.94	-.08
13	13	14	14	33073.86	.00	.00
14	13	15	14	33073.41	.00	.00
15	13	16	14	33072.97	.00	.00
16	13	17	14	33072.53	.00	.00
17	13	18	14	33072.11	.00	.00
18	13	19	14	33071.69	.00	.00
19	13	20	14	33071.28	.00	.00
20	13	21	14	33070.88	.00	.00
21	13	22	14	33070.48	.00	.00
22	13	23	14	33070.09	.00	.00
23	13	24	14	33069.71	.00	.00
15	15	16	16	33057.07	.00	.00
16	15	17	16	33056.64	.00	.00
17	15	18	16	33056.21	.00	.00
18	15	19	16	33055.80	.00	.00
19	15	20	16	33055.39	.00	.00
20	15	21	16	33054.99	.00	.00
21	15	22	16	33054.59	.00	.00
22	15	23	16	33054.21	.00	.00
23	15	24	16	33053.83	.00	.00
24	15	25	16	33053.46	.00	.00
25	15	26	16	33053.10	.00	.00
17	17	18	18	33038.98	.00	.00
18	17	19	18	33038.56	.00	.00
19	17	20	18	33038.15	.00	.00
20	17	21	18	33037.75	.00	.00
21	17	22	18	33037.36	.00	.00
22	17	23	18	33036.98	.00	.00
23	17	24	18	33036.60	.00	.00
24	17	25	18	33036.23	.00	.00
25	17	26	18	33035.87	.00	.00
26	17	27	18	33035.52	.00	.00
27	17	28	18	33035.17	.00	.00
19	19	20	20	33019.58	.00	.00
20	19	21	20	33019.18	.00	.00
21	19	22	20	33018.79	.00	.00
22	19	23	20	33018.40	.00	.00
23	19	24	20	33018.03	.00	.00
24	19	25	20	33017.66	.00	.00
25	19	26	20	33017.30	.00	.00
26	19	27	20	33016.95	.00	.00

Table 14. (Continued).

27	19	28	20	33016.61	.00	.00
28	19	29	20	33016.27	.00	.00
29	19	30	20	33015.94	.00	.00

* * * * * * * * R BRANCH * * * * * * * *

J'	K'	J"	K"	FREQ CALC	OBSERVED	DIFFERENCE
1	1	0	0	33155.40	.00	.00
2	1	1	0	33156.55	.00	.00
3	1	2	0	33156.58	.00	.00
4	1	3	0	33160.60	.00	.00
5	1	4	0	33157.81	.00	.00
6	1	5	0	33166.96	.00	.00
7	1	6	0	33159.11	.00	.00
8	1	7	0	33175.62	.00	.00
9	1	8	0	33160.51	.00	.00
10	1	9	0	33186.60	.00	.00
11	1	10	0	33162.06	.00	.00
3	3	2	2	33161.76	.00	.00
4	3	3	2	33162.36	33162.41	.05
5	3	4	2	33162.96	33162.86	-.11
6	3	5	2	33163.60	33163.40	-.20
7	3	6	2	33164.18	33164.20	.02
8	3	7	2	33164.88	33164.85	-.03
9	3	8	2	33165.37	33165.10	-.27
10	3	9	2	33166.21	33166.23	.02
11	3	10	2	33166.50	33166.50	-.00
12	3	11	2	33167.60	33167.62	.02
13	3	12	2	33167.56	33167.50	-.06
5	5	4	4	33166.81	33166.80	-.01
6	5	5	4	33167.43	33167.48	.05
7	5	6	4	33168.06	33168.05	-.01
8	5	7	4	33168.69	33168.71	.02
9	5	8	4	33169.34	33169.32	-.01
10	5	9	4	33169.98	.00	.00
11	5	10	4	33170.64	.00	.00
12	5	11	4	33171.30	.00	.00
13	5	12	4	33171.97	33172.00	.03
14	5	13	4	33172.64	33172.67	.03
15	5	14	4	33173.31	.00	.00
7	7	6	6	33170.56	33170.65	.09
8	7	7	6	33171.20	.00	.00
9	7	8	6	33171.84	.00	.00
10	7	9	6	33172.49	33172.41	-.08
11	7	10	6	33173.15	.00	.00
12	7	11	6	33173.82	33173.75	-.07
13	7	12	6	33174.50	33174.40	-.10
14	7	13	6	33175.18	.00	.00
15	7	14	6	33175.87	.00	.00
16	7	15	6	33176.56	.00	.00
17	7	16	6	33177.26	.00	.00
9	9	8	8	33173.00	33173.10	.10
10	9	9	8	33173.65	33173.55	-.10
11	9	10	8	33174.32	33174.41	.10
12	9	11	8	33174.99	33175.30	.31
13	9	12	8	33175.66	33175.90	.24

Table 14. (Continued).

14	9	13	8	33176.35	.00	.00
15	9	14	8	33177.04	33177.22	.18
16	9	15	8	33177.74	33177.58	-.16
17	9	16	8	33178.45	33178.50	.05
18	9	17	8	33179.16	33179.07	-.09
19	9	18	8	33179.88	.00	.00
11	11	10	10	33174.14	33174.00	-.14
12	11	11	10	33174.81	.00	.00
13	11	12	10	33175.49	33175.30	-.19
14	11	13	10	33176.17	33176.10	-.07
15	11	14	10	33176.87	33176.80	-.07
16	11	15	10	33177.57	33177.58	.01
17	11	16	10	33178.28	33178.29	.01
18	11	17	10	33179.00	33179.06	.06
19	11	18	10	33179.72	.00	.00
20	11	19	10	33180.46	33180.50	.04
21	11	20	10	33181.20	33181.07	-.13
13	13	12	12	33173.97	.00	.00
14	13	13	12	33174.65	.00	.00
15	13	14	12	33175.35	.00	.00
16	13	15	12	33176.05	.00	.00
17	13	16	12	33176.77	.00	.00
18	13	17	12	33177.49	.00	.00
19	13	18	12	33178.21	.00	.00
20	13	19	12	33178.95	.00	.00
21	13	20	12	33179.69	.00	.00
22	13	21	12	33180.44	.00	.00
23	13	22	12	33181.20	.00	.00
15	15	14	14	33172.49	.00	.00
16	15	15	14	33173.19	.00	.00
17	15	16	14	33173.91	.00	.00
18	15	17	14	33174.63	.00	.00
19	15	18	14	33175.36	.00	.00
20	15	19	14	33176.10	.00	.00
21	15	20	14	33176.84	.00	.00
22	15	21	14	33177.59	.00	.00
23	15	22	14	33178.35	.00	.00
24	15	23	14	33179.12	.00	.00
25	15	24	14	33179.90	.00	.00
17	17	16	16	33169.71	.00	.00
18	17	17	16	33170.43	.00	.00
19	17	18	16	33171.16	.00	.00
20	17	19	16	33171.90	.00	.00
21	17	20	16	33172.64	.00	.00
22	17	21	16	33173.40	.00	.00
23	17	22	16	33174.16	.00	.00
24	17	23	16	33174.93	.00	.00
25	17	24	16	33175.71	.00	.00
26	17	25	16	33176.49	.00	.00
27	17	26	16	33177.29	.00	.00
19	19	18	18	33165.62	.00	.00
20	19	19	18	33166.36	.00	.00
21	19	20	18	33167.11	.00	.00
22	19	21	18	33167.86	.00	.00
23	19	22	18	33168.62	.00	.00

Table 14. (Continued).

24	19	23	18	33169.40	.00	.00
25	19	24	18	33170.18	.00	.00
26	19	25	18	33170.96	.00	.00
27	19	26	18	33171.76	.00	.00
28	19	27	18	33172.56	.00	.00
29	19	28	18	33173.37	.00	.00

APPENDIX IV

OBSERVED SPECTRA

This Appendix presents densitometer traces of the observed magnetic rotation spectra of SO_2^{16} and SO_2^{18}. Figures 17 through 27 were generated by the program MPLOT described in Appendix I. Figures 28 and 29 illustrate plotter output characteristic of the programs SCAN and XPAND.

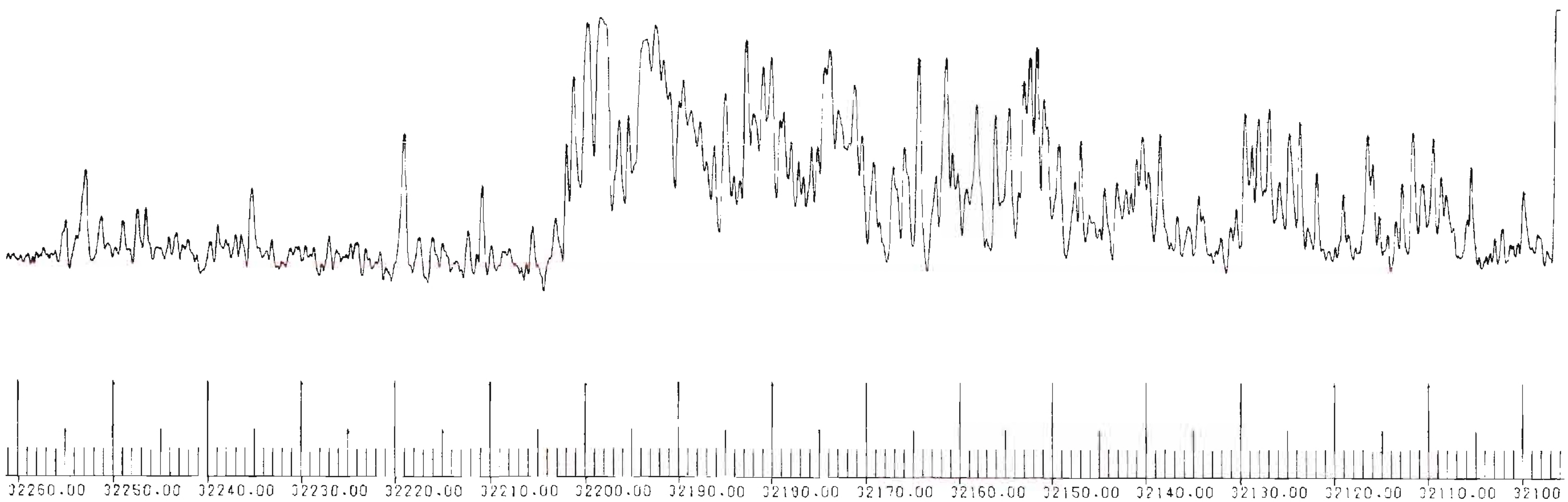


Fig. 17. Magnetic Rotation Spectrum of the B Band of SO_2^{16}.

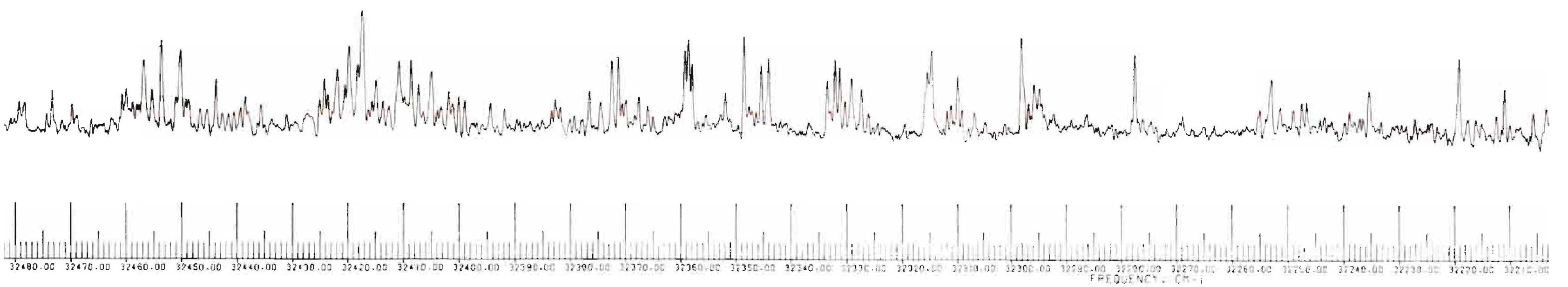


Fig. 18. Magnetic Rotation Spectrum of the C Band of SO_2^{16}.

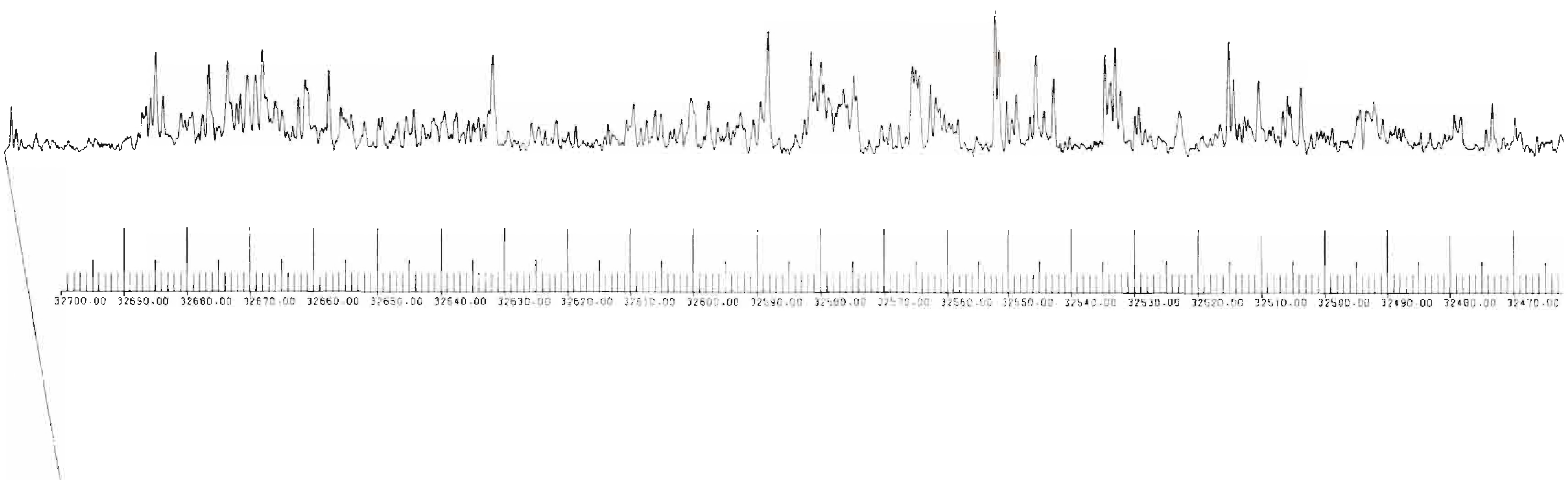


Fig. 19. Magnetic Rotation Spectrum of the D Band of SO_2^{16}.

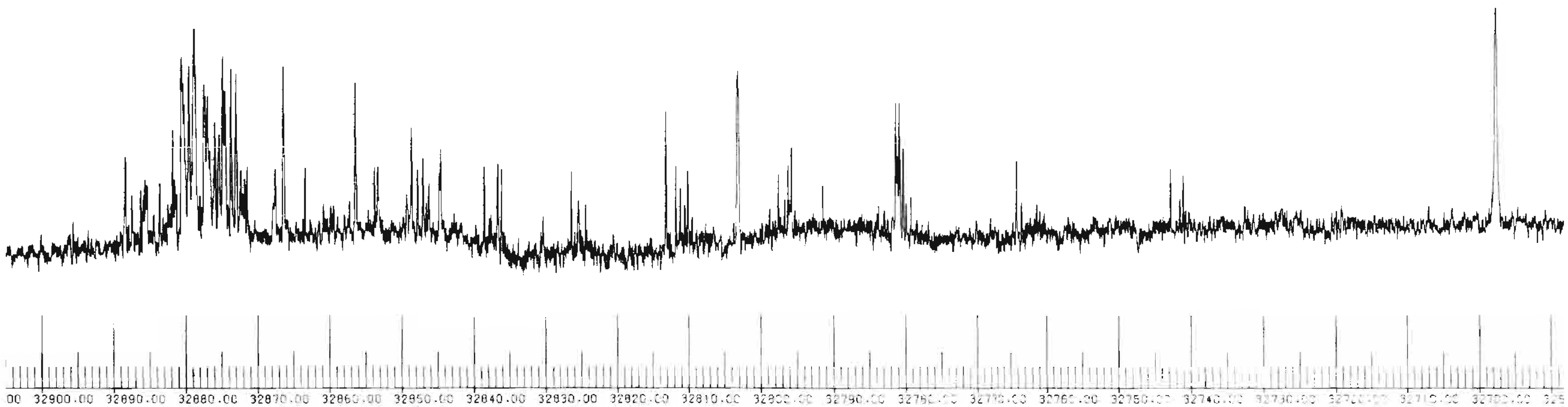


Fig. 20. Magnetic Rotation Spectrum of the E Band of SO_2^{16}.

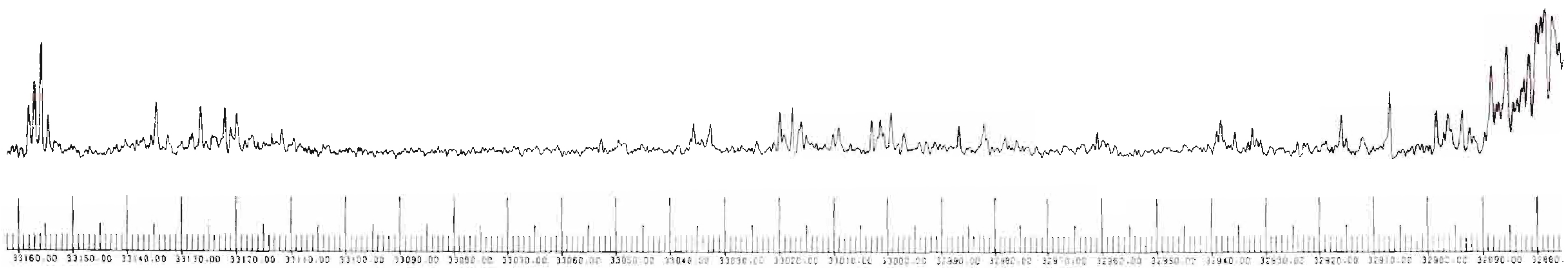


Fig. 21. Magnetic Rotation Spectrum of the F Band of SO_2^{16}.

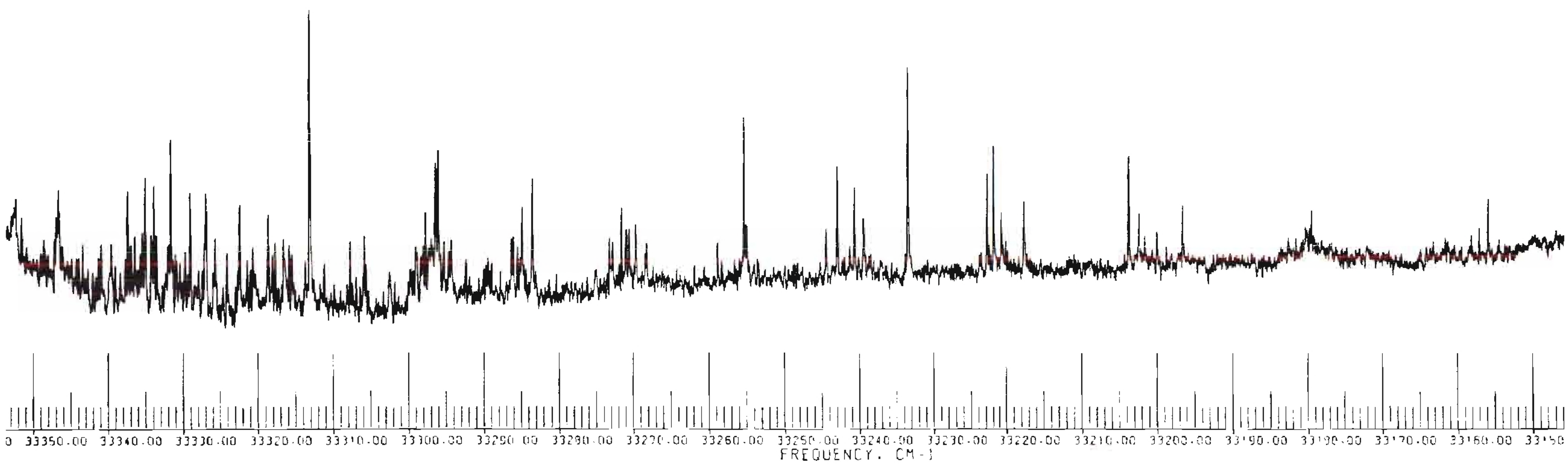


Fig. 22. Magnetic Rotation Spectrum of the G Band of SO_2^{16}.

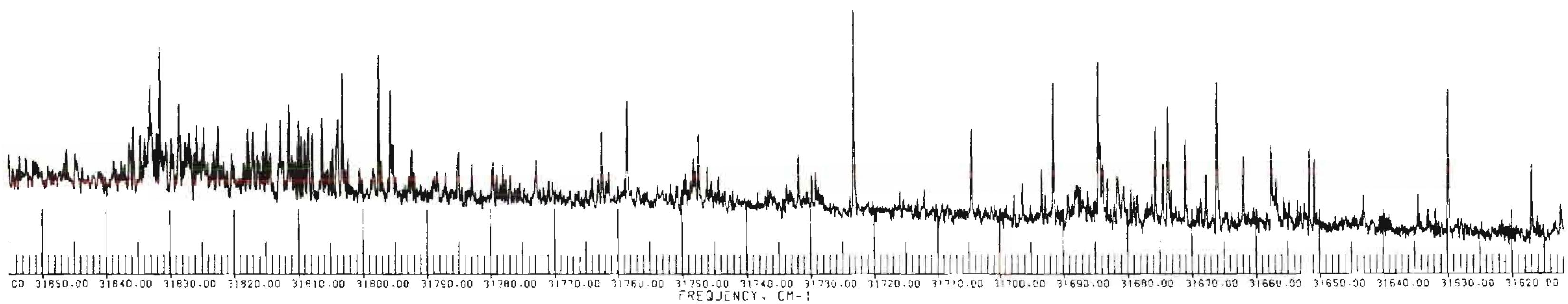


Fig. 23. Magnetic Rotation Spectrum of the A Band of SO_2^{18}.

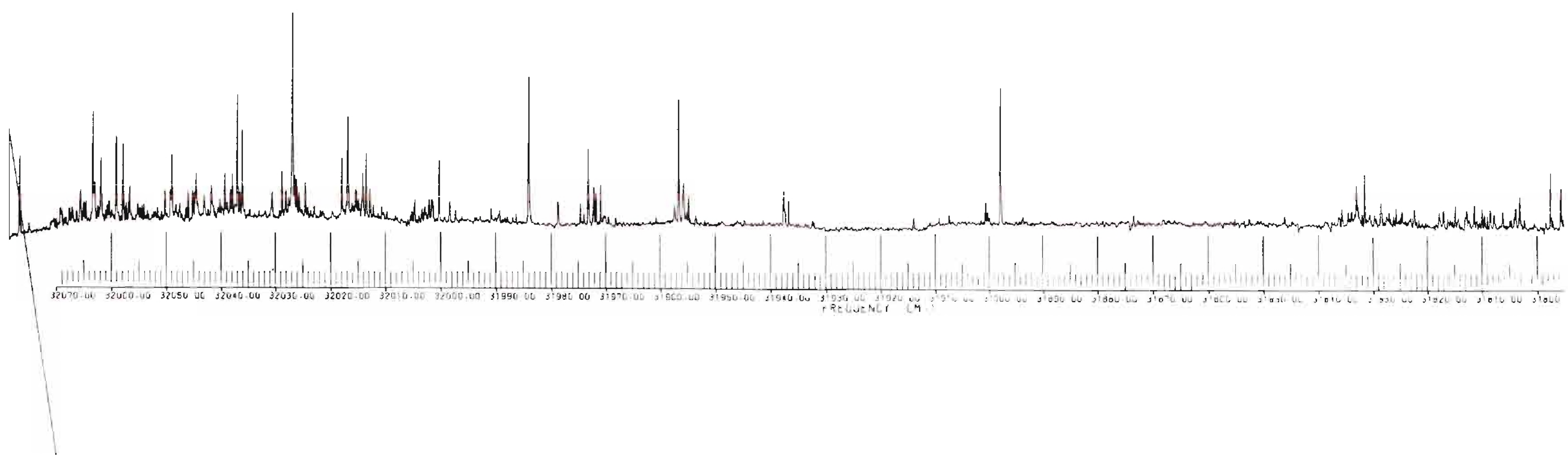


Fig. 24. Magnetic Rotation Spectrum of the B Band of SO_2^{18}.

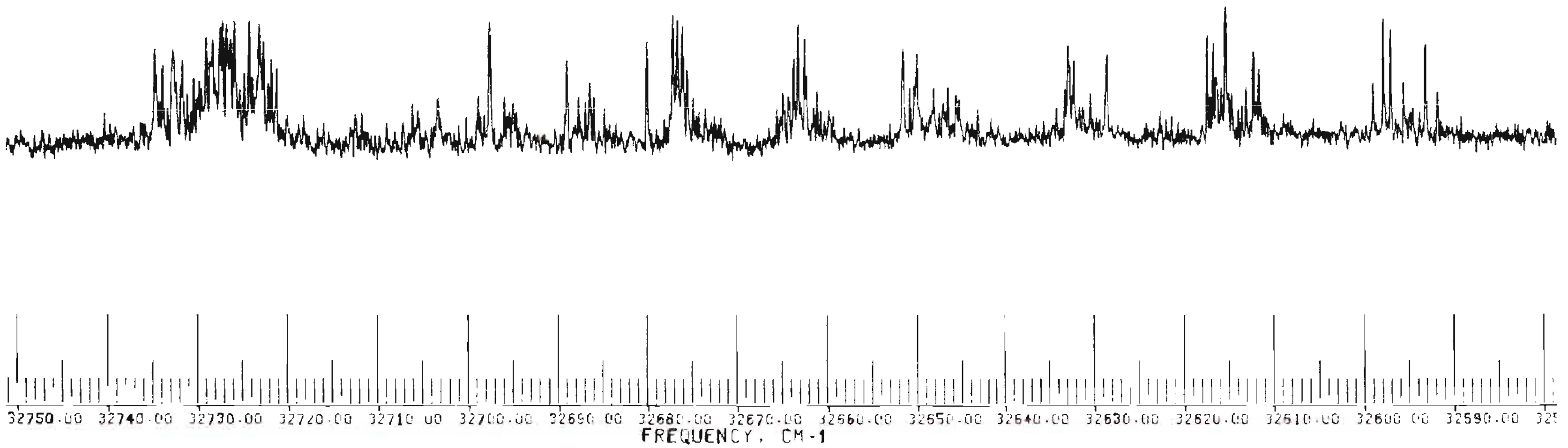


Fig. 25. Magnetic Rotation Spectrum of the E Band of SO_2^{18}.

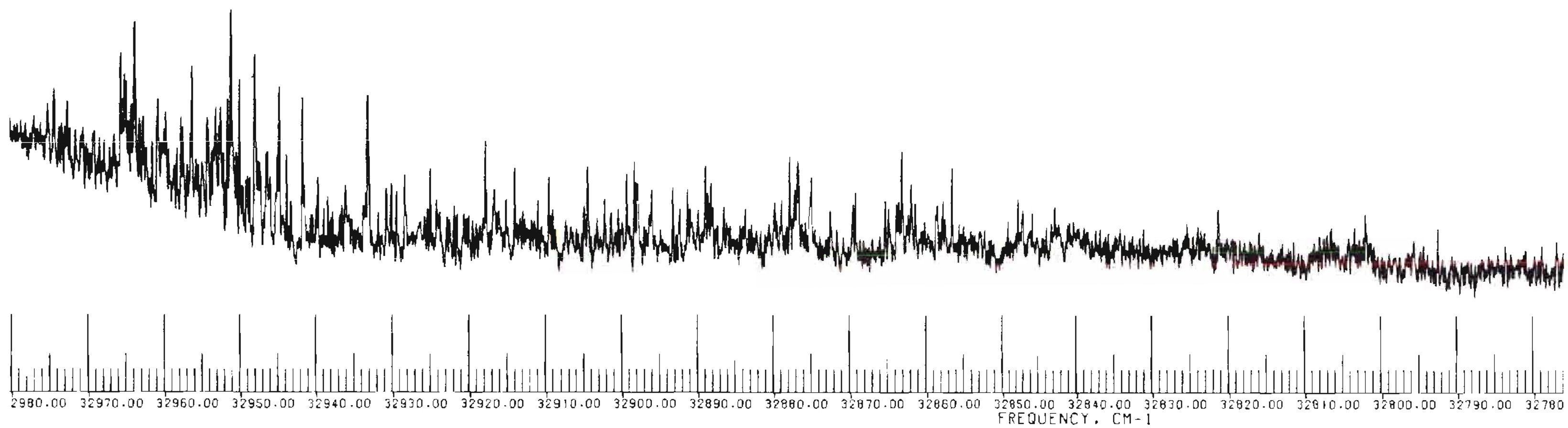


Fig. 26. Magnetic Rotation Spectrum of the F Band of SO_2^{18}.

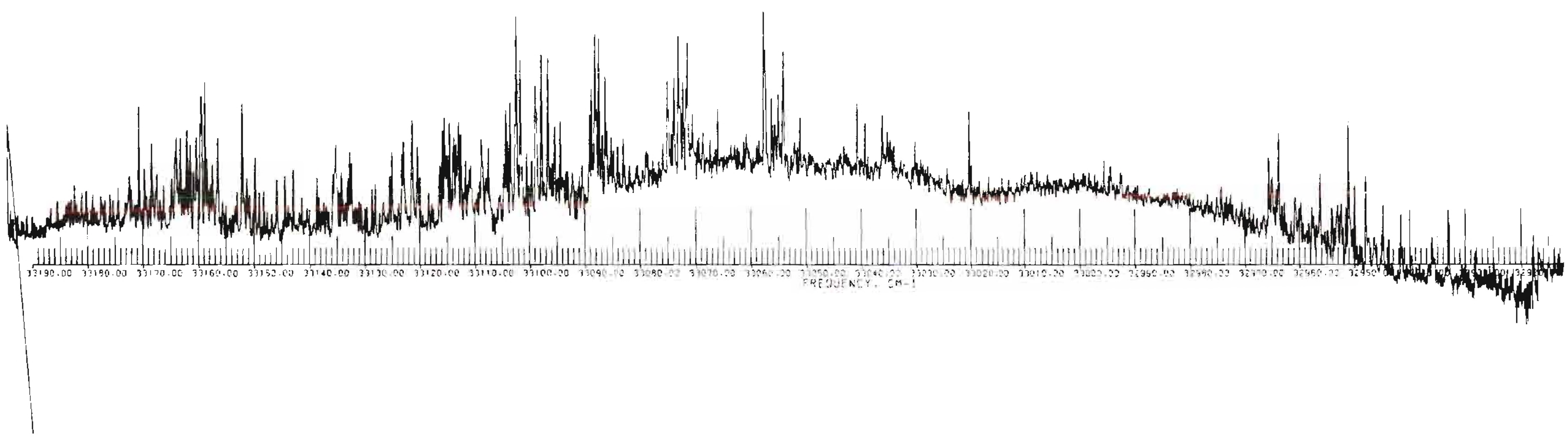


Fig. 27. Magnetic Rotation Spectrum of the G Band of SO_2^{18}.

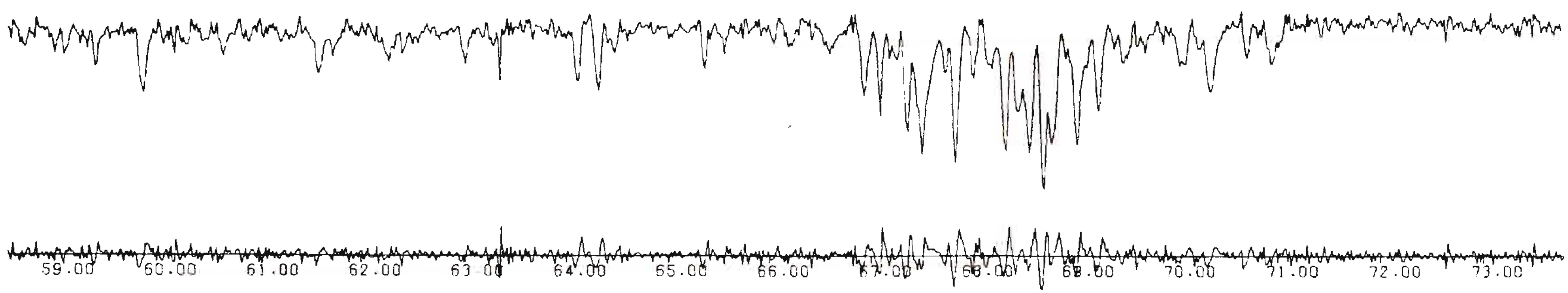


Fig. 28. Characteristic Output of the Program SCAN.

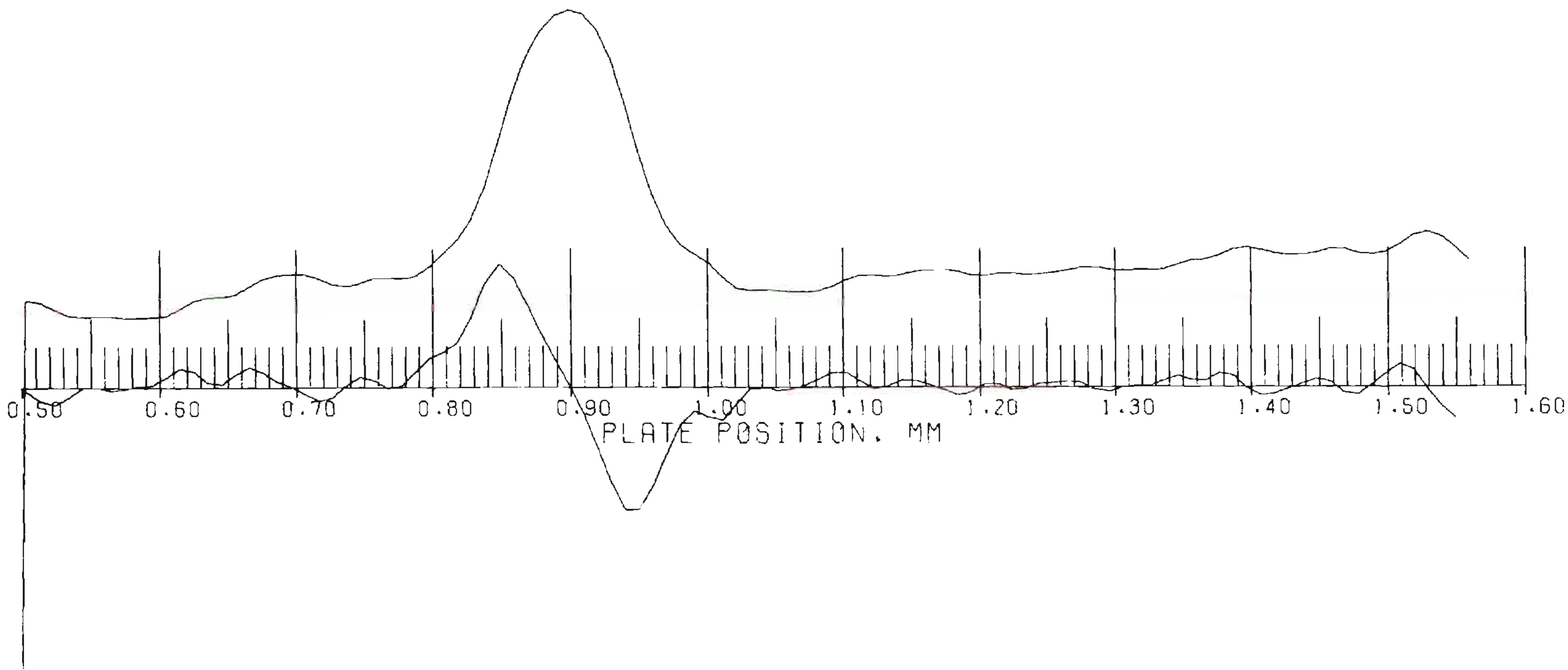


Fig. 29. Characteristic Output of the Program XPAND.

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